Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 05:02 PM JST

PDB ID	:	26IP / pdb_000026ip
EMDB ID	:	EMD-80684
Title	:	Structure of recombinant RyR2 in the closed state (EGTA dataset)
Authors	:	Otori, Y.; Takeuchi, S.; Ogawa, H.
Deposited on	:	2026-05-01
Resolution	:	2.83 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

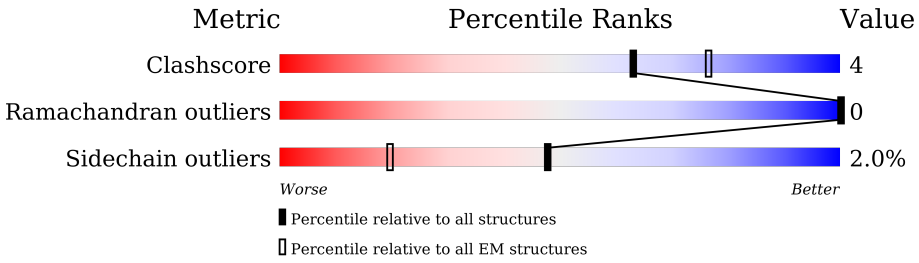
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

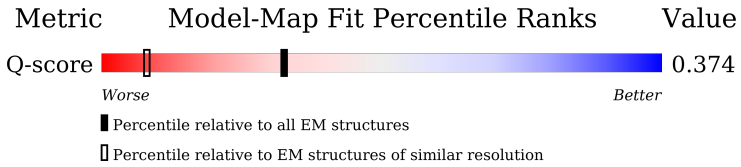
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4966	25% 75% 10% 15%
1	B	4966	25% 75% 10% 15%
1	C	4966	25% 75% 10% 15%
1	D	4966	25% 75% 10% 15%

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Mol	Chain	Length	Quality of chain
2	G	176	
2	H	176	
2	I	176	
2	J	176	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 275096 atoms, of which 136804 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4218	Total	C	H	N	O	S	0	0
			67133	21510	33380	5735	6281	227		
1	B	4218	Total	C	H	N	O	S	0	0
			67133	21510	33380	5735	6281	227		
1	C	4218	Total	C	H	N	O	S	0	0
			67133	21510	33380	5735	6281	227		
1	D	4218	Total	C	H	N	O	S	0	0
			67133	21510	33380	5735	6281	227		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	G	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		
2	H	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		
2	I	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		
2	J	107	Total	C	H	N	O	S	0	0
			1640	516	821	144	155	4		

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-67	MET	-	initiating methionine	UNP P68106
G	-66	GLY	-	expression tag	UNP P68106
G	-65	SER	-	expression tag	UNP P68106
G	-64	SER	-	expression tag	UNP P68106
G	-63	HIS	-	expression tag	UNP P68106
G	-62	HIS	-	expression tag	UNP P68106
G	-61	HIS	-	expression tag	UNP P68106
G	-60	HIS	-	expression tag	UNP P68106
G	-59	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-58	HIS	-	expression tag	UNP P68106
G	-57	SER	-	expression tag	UNP P68106
G	-56	SER	-	expression tag	UNP P68106
G	-55	GLY	-	expression tag	UNP P68106
G	-54	LEU	-	expression tag	UNP P68106
G	-53	VAL	-	expression tag	UNP P68106
G	-52	PRO	-	expression tag	UNP P68106
G	-51	ARG	-	expression tag	UNP P68106
G	-50	GLY	-	expression tag	UNP P68106
G	-49	SER	-	expression tag	UNP P68106
G	-48	HIS	-	expression tag	UNP P68106
G	-47	MET	-	expression tag	UNP P68106
G	-46	ALA	-	expression tag	UNP P68106
G	-45	SER	-	expression tag	UNP P68106
G	-44	MET	-	expression tag	UNP P68106
G	-43	ASP	-	expression tag	UNP P68106
G	-42	GLU	-	expression tag	UNP P68106
G	-41	LYS	-	expression tag	UNP P68106
G	-40	THR	-	expression tag	UNP P68106
G	-39	THR	-	expression tag	UNP P68106
G	-38	GLY	-	expression tag	UNP P68106
G	-37	TRP	-	expression tag	UNP P68106
G	-36	ARG	-	expression tag	UNP P68106
G	-35	GLY	-	expression tag	UNP P68106
G	-34	GLY	-	expression tag	UNP P68106
G	-33	HIS	-	expression tag	UNP P68106
G	-32	VAL	-	expression tag	UNP P68106
G	-31	VAL	-	expression tag	UNP P68106
G	-30	GLU	-	expression tag	UNP P68106
G	-29	GLY	-	expression tag	UNP P68106
G	-28	LEU	-	expression tag	UNP P68106
G	-27	ALA	-	expression tag	UNP P68106
G	-26	GLY	-	expression tag	UNP P68106
G	-25	GLU	-	expression tag	UNP P68106
G	-24	LEU	-	expression tag	UNP P68106
G	-23	GLU	-	expression tag	UNP P68106
G	-22	GLN	-	expression tag	UNP P68106
G	-21	LEU	-	expression tag	UNP P68106
G	-20	ARG	-	expression tag	UNP P68106
G	-19	ALA	-	expression tag	UNP P68106
G	-18	ARG	-	expression tag	UNP P68106
G	-17	LEU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-16	GLU	-	expression tag	UNP P68106
G	-15	HIS	-	expression tag	UNP P68106
G	-14	HIS	-	expression tag	UNP P68106
G	-13	PRO	-	expression tag	UNP P68106
G	-12	GLN	-	expression tag	UNP P68106
G	-11	GLY	-	expression tag	UNP P68106
G	-10	GLN	-	expression tag	UNP P68106
G	-9	ARG	-	expression tag	UNP P68106
G	-8	GLU	-	expression tag	UNP P68106
G	-7	PRO	-	expression tag	UNP P68106
G	-6	GLY	-	expression tag	UNP P68106
G	-5	SER	-	expression tag	UNP P68106
G	-4	GLY	-	expression tag	UNP P68106
G	-3	GLY	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	GLY	-	expression tag	UNP P68106
G	0	GLY	-	expression tag	UNP P68106
G	1	THR	-	expression tag	UNP P68106
H	-67	MET	-	initiating methionine	UNP P68106
H	-66	GLY	-	expression tag	UNP P68106
H	-65	SER	-	expression tag	UNP P68106
H	-64	SER	-	expression tag	UNP P68106
H	-63	HIS	-	expression tag	UNP P68106
H	-62	HIS	-	expression tag	UNP P68106
H	-61	HIS	-	expression tag	UNP P68106
H	-60	HIS	-	expression tag	UNP P68106
H	-59	HIS	-	expression tag	UNP P68106
H	-58	HIS	-	expression tag	UNP P68106
H	-57	SER	-	expression tag	UNP P68106
H	-56	SER	-	expression tag	UNP P68106
H	-55	GLY	-	expression tag	UNP P68106
H	-54	LEU	-	expression tag	UNP P68106
H	-53	VAL	-	expression tag	UNP P68106
H	-52	PRO	-	expression tag	UNP P68106
H	-51	ARG	-	expression tag	UNP P68106
H	-50	GLY	-	expression tag	UNP P68106
H	-49	SER	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	MET	-	expression tag	UNP P68106
H	-46	ALA	-	expression tag	UNP P68106
H	-45	SER	-	expression tag	UNP P68106
H	-44	MET	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-43	ASP	-	expression tag	UNP P68106
H	-42	GLU	-	expression tag	UNP P68106
H	-41	LYS	-	expression tag	UNP P68106
H	-40	THR	-	expression tag	UNP P68106
H	-39	THR	-	expression tag	UNP P68106
H	-38	GLY	-	expression tag	UNP P68106
H	-37	TRP	-	expression tag	UNP P68106
H	-36	ARG	-	expression tag	UNP P68106
H	-35	GLY	-	expression tag	UNP P68106
H	-34	GLY	-	expression tag	UNP P68106
H	-33	HIS	-	expression tag	UNP P68106
H	-32	VAL	-	expression tag	UNP P68106
H	-31	VAL	-	expression tag	UNP P68106
H	-30	GLU	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	LEU	-	expression tag	UNP P68106
H	-27	ALA	-	expression tag	UNP P68106
H	-26	GLY	-	expression tag	UNP P68106
H	-25	GLU	-	expression tag	UNP P68106
H	-24	LEU	-	expression tag	UNP P68106
H	-23	GLU	-	expression tag	UNP P68106
H	-22	GLN	-	expression tag	UNP P68106
H	-21	LEU	-	expression tag	UNP P68106
H	-20	ARG	-	expression tag	UNP P68106
H	-19	ALA	-	expression tag	UNP P68106
H	-18	ARG	-	expression tag	UNP P68106
H	-17	LEU	-	expression tag	UNP P68106
H	-16	GLU	-	expression tag	UNP P68106
H	-15	HIS	-	expression tag	UNP P68106
H	-14	HIS	-	expression tag	UNP P68106
H	-13	PRO	-	expression tag	UNP P68106
H	-12	GLN	-	expression tag	UNP P68106
H	-11	GLY	-	expression tag	UNP P68106
H	-10	GLN	-	expression tag	UNP P68106
H	-9	ARG	-	expression tag	UNP P68106
H	-8	GLU	-	expression tag	UNP P68106
H	-7	PRO	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	SER	-	expression tag	UNP P68106
H	-4	GLY	-	expression tag	UNP P68106
H	-3	GLY	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	expression tag	UNP P68106
H	0	GLY	-	expression tag	UNP P68106
H	1	THR	-	expression tag	UNP P68106
I	-67	MET	-	initiating methionine	UNP P68106
I	-66	GLY	-	expression tag	UNP P68106
I	-65	SER	-	expression tag	UNP P68106
I	-64	SER	-	expression tag	UNP P68106
I	-63	HIS	-	expression tag	UNP P68106
I	-62	HIS	-	expression tag	UNP P68106
I	-61	HIS	-	expression tag	UNP P68106
I	-60	HIS	-	expression tag	UNP P68106
I	-59	HIS	-	expression tag	UNP P68106
I	-58	HIS	-	expression tag	UNP P68106
I	-57	SER	-	expression tag	UNP P68106
I	-56	SER	-	expression tag	UNP P68106
I	-55	GLY	-	expression tag	UNP P68106
I	-54	LEU	-	expression tag	UNP P68106
I	-53	VAL	-	expression tag	UNP P68106
I	-52	PRO	-	expression tag	UNP P68106
I	-51	ARG	-	expression tag	UNP P68106
I	-50	GLY	-	expression tag	UNP P68106
I	-49	SER	-	expression tag	UNP P68106
I	-48	HIS	-	expression tag	UNP P68106
I	-47	MET	-	expression tag	UNP P68106
I	-46	ALA	-	expression tag	UNP P68106
I	-45	SER	-	expression tag	UNP P68106
I	-44	MET	-	expression tag	UNP P68106
I	-43	ASP	-	expression tag	UNP P68106
I	-42	GLU	-	expression tag	UNP P68106
I	-41	LYS	-	expression tag	UNP P68106
I	-40	THR	-	expression tag	UNP P68106
I	-39	THR	-	expression tag	UNP P68106
I	-38	GLY	-	expression tag	UNP P68106
I	-37	TRP	-	expression tag	UNP P68106
I	-36	ARG	-	expression tag	UNP P68106
I	-35	GLY	-	expression tag	UNP P68106
I	-34	GLY	-	expression tag	UNP P68106
I	-33	HIS	-	expression tag	UNP P68106
I	-32	VAL	-	expression tag	UNP P68106
I	-31	VAL	-	expression tag	UNP P68106
I	-30	GLU	-	expression tag	UNP P68106
I	-29	GLY	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-28	LEU	-	expression tag	UNP P68106
I	-27	ALA	-	expression tag	UNP P68106
I	-26	GLY	-	expression tag	UNP P68106
I	-25	GLU	-	expression tag	UNP P68106
I	-24	LEU	-	expression tag	UNP P68106
I	-23	GLU	-	expression tag	UNP P68106
I	-22	GLN	-	expression tag	UNP P68106
I	-21	LEU	-	expression tag	UNP P68106
I	-20	ARG	-	expression tag	UNP P68106
I	-19	ALA	-	expression tag	UNP P68106
I	-18	ARG	-	expression tag	UNP P68106
I	-17	LEU	-	expression tag	UNP P68106
I	-16	GLU	-	expression tag	UNP P68106
I	-15	HIS	-	expression tag	UNP P68106
I	-14	HIS	-	expression tag	UNP P68106
I	-13	PRO	-	expression tag	UNP P68106
I	-12	GLN	-	expression tag	UNP P68106
I	-11	GLY	-	expression tag	UNP P68106
I	-10	GLN	-	expression tag	UNP P68106
I	-9	ARG	-	expression tag	UNP P68106
I	-8	GLU	-	expression tag	UNP P68106
I	-7	PRO	-	expression tag	UNP P68106
I	-6	GLY	-	expression tag	UNP P68106
I	-5	SER	-	expression tag	UNP P68106
I	-4	GLY	-	expression tag	UNP P68106
I	-3	GLY	-	expression tag	UNP P68106
I	-2	SER	-	expression tag	UNP P68106
I	-1	GLY	-	expression tag	UNP P68106
I	0	GLY	-	expression tag	UNP P68106
I	1	THR	-	expression tag	UNP P68106
J	-67	MET	-	initiating methionine	UNP P68106
J	-66	GLY	-	expression tag	UNP P68106
J	-65	SER	-	expression tag	UNP P68106
J	-64	SER	-	expression tag	UNP P68106
J	-63	HIS	-	expression tag	UNP P68106
J	-62	HIS	-	expression tag	UNP P68106
J	-61	HIS	-	expression tag	UNP P68106
J	-60	HIS	-	expression tag	UNP P68106
J	-59	HIS	-	expression tag	UNP P68106
J	-58	HIS	-	expression tag	UNP P68106
J	-57	SER	-	expression tag	UNP P68106
J	-56	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-55	GLY	-	expression tag	UNP P68106
J	-54	LEU	-	expression tag	UNP P68106
J	-53	VAL	-	expression tag	UNP P68106
J	-52	PRO	-	expression tag	UNP P68106
J	-51	ARG	-	expression tag	UNP P68106
J	-50	GLY	-	expression tag	UNP P68106
J	-49	SER	-	expression tag	UNP P68106
J	-48	HIS	-	expression tag	UNP P68106
J	-47	MET	-	expression tag	UNP P68106
J	-46	ALA	-	expression tag	UNP P68106
J	-45	SER	-	expression tag	UNP P68106
J	-44	MET	-	expression tag	UNP P68106
J	-43	ASP	-	expression tag	UNP P68106
J	-42	GLU	-	expression tag	UNP P68106
J	-41	LYS	-	expression tag	UNP P68106
J	-40	THR	-	expression tag	UNP P68106
J	-39	THR	-	expression tag	UNP P68106
J	-38	GLY	-	expression tag	UNP P68106
J	-37	TRP	-	expression tag	UNP P68106
J	-36	ARG	-	expression tag	UNP P68106
J	-35	GLY	-	expression tag	UNP P68106
J	-34	GLY	-	expression tag	UNP P68106
J	-33	HIS	-	expression tag	UNP P68106
J	-32	VAL	-	expression tag	UNP P68106
J	-31	VAL	-	expression tag	UNP P68106
J	-30	GLU	-	expression tag	UNP P68106
J	-29	GLY	-	expression tag	UNP P68106
J	-28	LEU	-	expression tag	UNP P68106
J	-27	ALA	-	expression tag	UNP P68106
J	-26	GLY	-	expression tag	UNP P68106
J	-25	GLU	-	expression tag	UNP P68106
J	-24	LEU	-	expression tag	UNP P68106
J	-23	GLU	-	expression tag	UNP P68106
J	-22	GLN	-	expression tag	UNP P68106
J	-21	LEU	-	expression tag	UNP P68106
J	-20	ARG	-	expression tag	UNP P68106
J	-19	ALA	-	expression tag	UNP P68106
J	-18	ARG	-	expression tag	UNP P68106
J	-17	LEU	-	expression tag	UNP P68106
J	-16	GLU	-	expression tag	UNP P68106
J	-15	HIS	-	expression tag	UNP P68106
J	-14	HIS	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	PRO	-	expression tag	UNP P68106
J	-12	GLN	-	expression tag	UNP P68106
J	-11	GLY	-	expression tag	UNP P68106
J	-10	GLN	-	expression tag	UNP P68106
J	-9	ARG	-	expression tag	UNP P68106
J	-8	GLU	-	expression tag	UNP P68106
J	-7	PRO	-	expression tag	UNP P68106
J	-6	GLY	-	expression tag	UNP P68106
J	-5	SER	-	expression tag	UNP P68106
J	-4	GLY	-	expression tag	UNP P68106
J	-3	GLY	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	GLY	-	expression tag	UNP P68106
J	0	GLY	-	expression tag	UNP P68106
J	1	THR	-	expression tag	UNP P68106

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

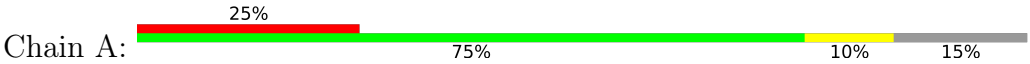
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Zn 1 1	0
3	B	1	Total Zn 1 1	0
3	C	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0

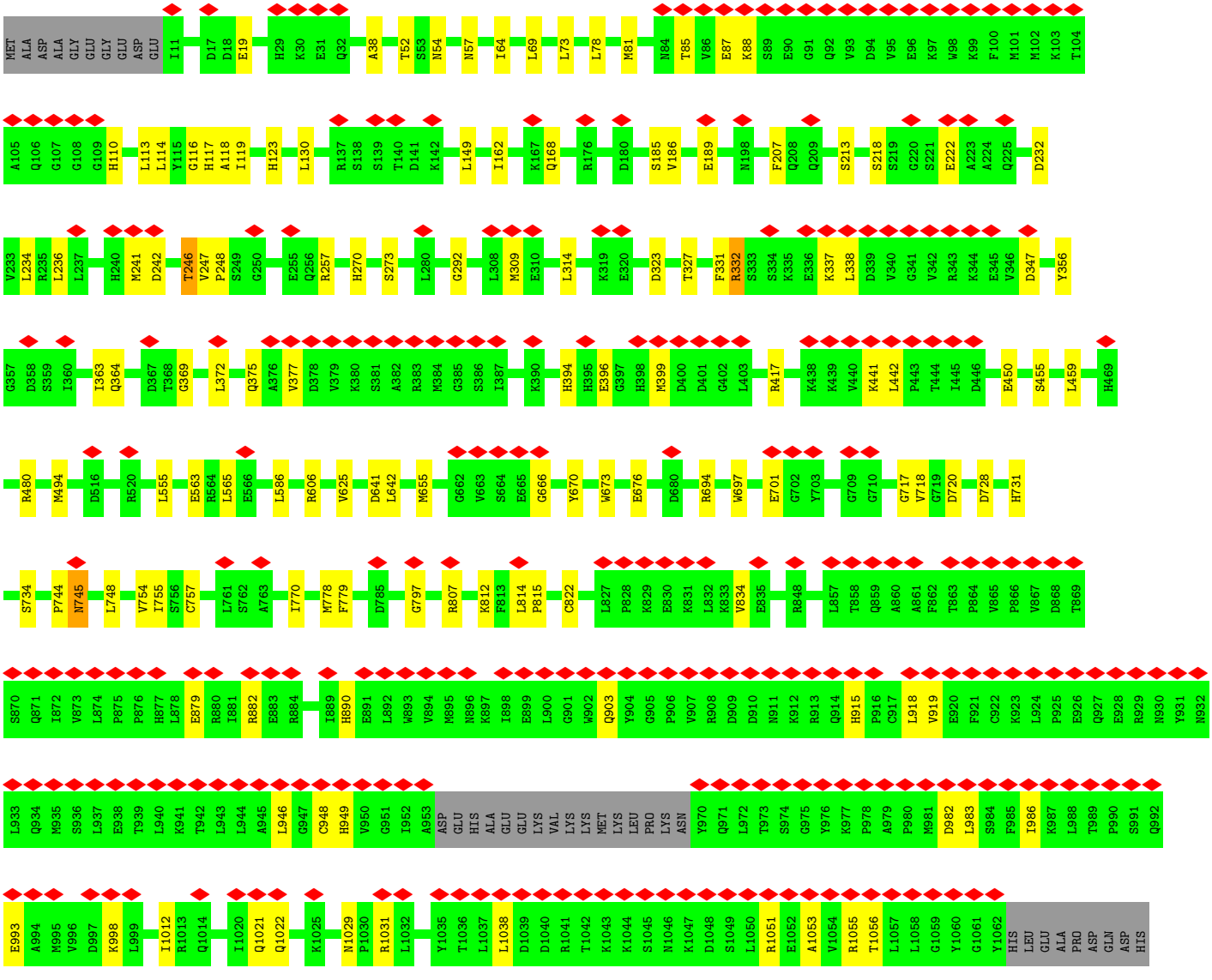
3 Residue-property plots (i)

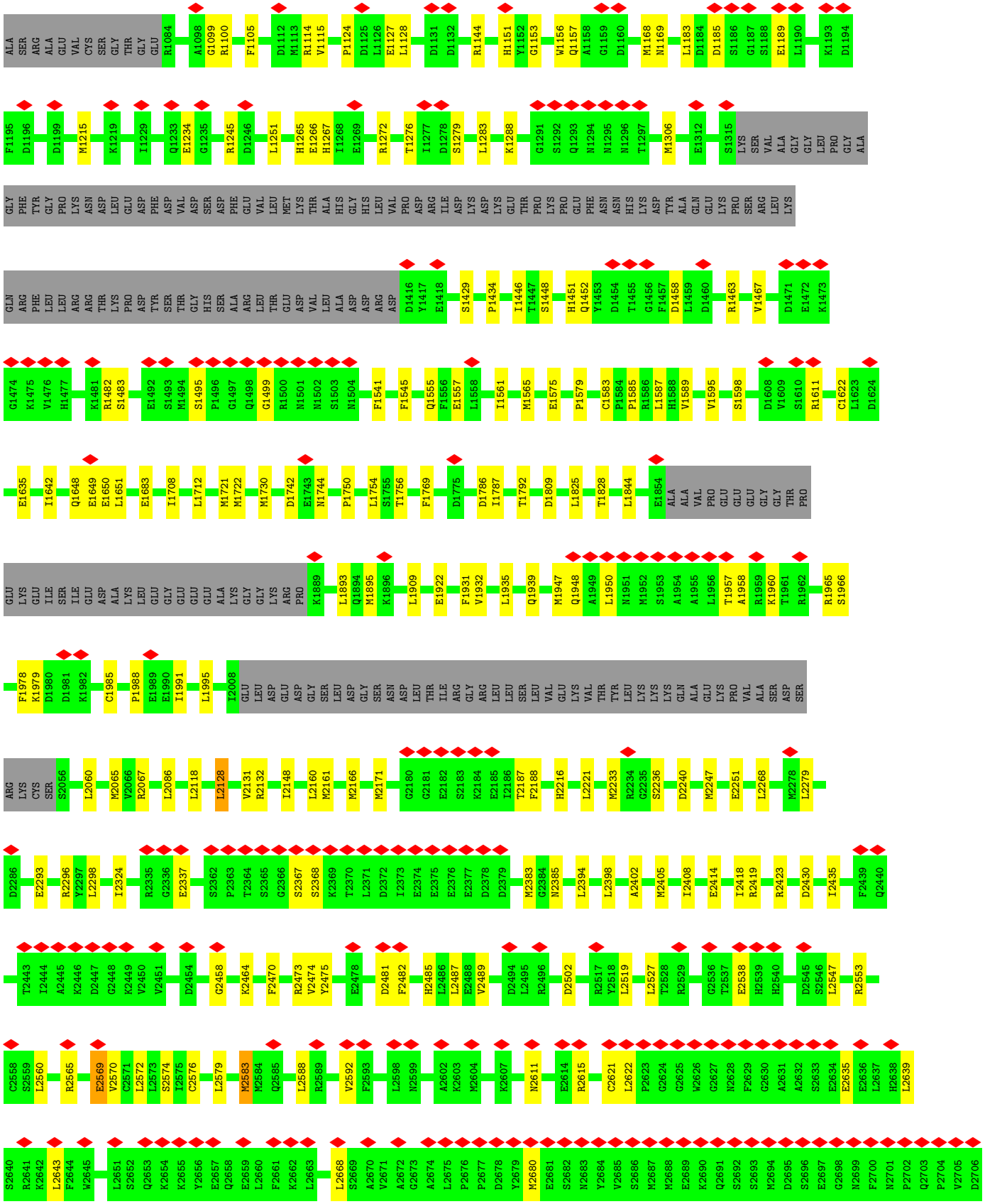
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

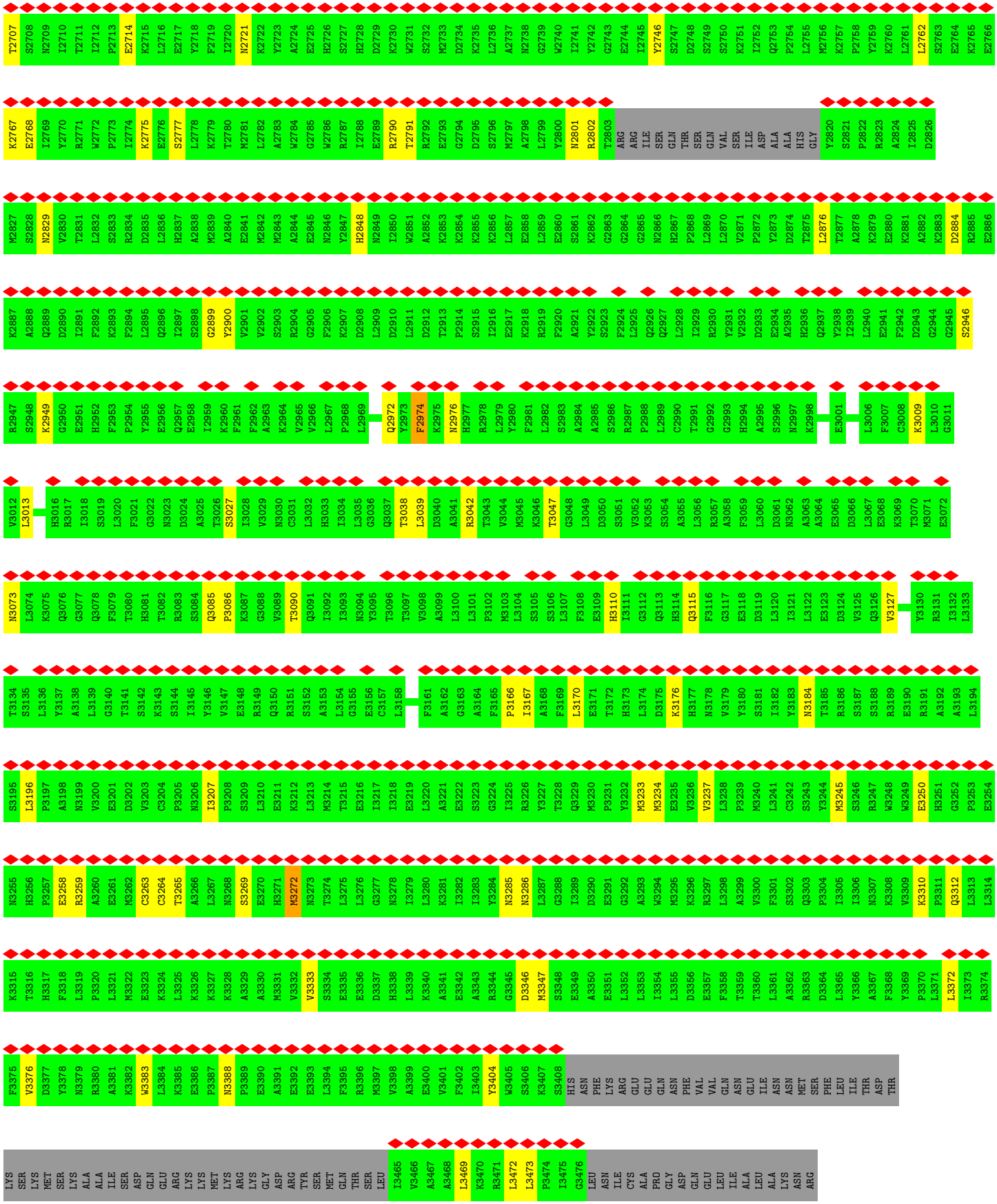
- Molecule 1: Ryanodine receptor 2

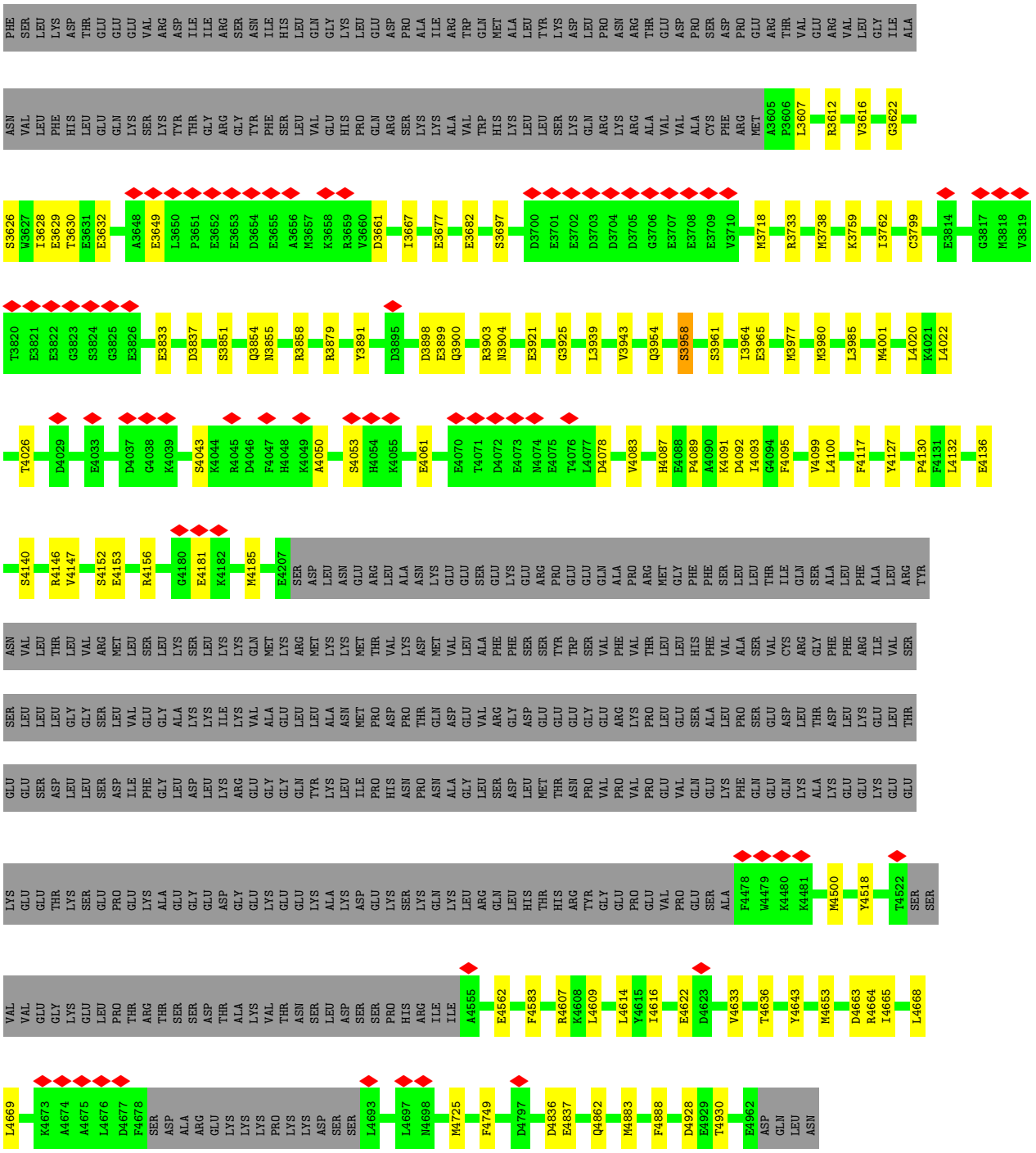
Chain A:






ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 A1098 G1099 R1100 F1105 D1112 M1113 R1114 V1115 P1124 D1125 L1126 E1127 L1128 D1131 D1132 R1144 H1151 Y1152 G1153 W1156 Q1157 A1158 G1159 D1160 M1168 N1169 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190 K1193 D1194
F1195 D1196 D1199 M1215 K1219 I1229 Q1233 E1234 G1235 R1245 D1246 L1251 H1265 E1266 H1267 I1268 E1269 R1272 T1276 I1277 D1278 S1279 L1283 K1288 G1291 S1292 Q1293 N1294 N1295 N1296 T1297 M1306 E1312 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY ALA
GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS
GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1417 E1418 S1429 P1434 I1446 T1447 S1448 H1451 Q1452 Y1453 D1454 T1455 G1456 F1457 D1458 L1459 D1460 R1463 V1467 D1471 E1472 K1473
G1474 K1475 V1476 H1477 K1481 R1482 S1483 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 S1503 N1504 F1541 F1545 Q1555 F1556 E1557 L1558 I1561 M1565 E1575 P1579 C1583 P1584 P1585 R1586 L1587 H1588 V1589 V1595 S1598 D1608 V1609 S1610 R1611 C1622 L1623 D1624
E1635 I1642 Q1648 E1649 E1650 L1651 E1683 I1708 L1712 M1721 M1722 M1730 D1742 E1743 N1744 P1750 L1754 S1755 T1756 F1769 D1775 D1786 I1787 T1792 D1809 L1825 T1828 L1844 E1854 ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO
GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 L1893 Q1894 M1895 K1896 L1909 E1922 F1931 V1932 L1935 Q1939 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 R1965 S1966
F1978 K1979 D1980 D1981 K1982 C1985 P1988 E1989 E1990 I1991 L1995 I2008 GLU LEU ASP GLU ASP GLY SER LEU LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER
ARG LYS CYS SER S2056 L2060 M2065 V2066 R2067 L2086 L2118 L2128 V2131 R2132 I2148 L2160 M2161 M2166 M2171 G2180 G2181 E2182 S2183 K2184 E2185 I2186 T2187 F2188 H2216 L2221 M2233 R2234 G2235 S2236 D2240 M2247 E2251 L2268 M2278 L2279
D2286 E2293 R2296 Y2297 L2298 I2324 R2335 G2336 E2337 S2362 P2363 T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 M2383 G2384 N2385 L2394 L2398 A2402 M2405 I2408 E2414 I2418 R2419 R2423 D2430 I2435 F2439 Q2440
T2443 I2444 A2445 K2446 D2447 G2448 K2449 V2450 V2451 D2454 G2458 K2464 F2470 R2473 V2474 Y2475 E2478 D2481 F2482 H2485 L2486 L2487 E2488 V2489 D2494 L2495 R2496 D2502 R2517 Y2518 L2519 L2527 T2528 R2529 G2536 T2537 E2538 H2539 H2540 D2545 S2546 L2547 R2553
C2558 S2559 L2560 R2565 E2569 V2570 C2571 L2572 L2573 S2574 I2575 C2576 L2579 M2583 M2584 Q2585 L2588 R2589 V2592 F2693 L2698 N2599 A2602 K2603 M2604 K2607 N2611 E2614 R2615 C2621 L2622 P2623 G2624 G2625 W2626 G2627 N2628 F2629 G2630 A2631 A2632 S2633 E2634 E2635 E2636 L2637 H2638 L2639
S2640 R2641 K2642 L2643 F2644 W2645 L2651 S2652 Q2653 K2654 K2655 Y2656 E2657 Q2658 E2659 L2660 F2661 K2662 L2663 L2668 S2669 A2670 V2671 A2672 G2673 A2674 L2675 P2676 P2677 D2678 Y2679 M2680 E2681 S2682 N2683 Y2684 V2685 S2686 M2687 M2688 E2689 K2690 Q2691 S2692 S2693 M2694 D2695 S2696 E2697 G2698 N2699 P2700 N2701 P2702 Q2703 P2704 V2705 D2706

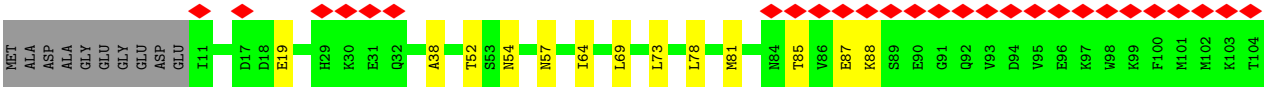

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K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775 E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 R2802 T2803 ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY Y2820 S2821 P2822 R2823 A2824 I2825 D2826
M2827 S2828 N2829 Y2830 T2831 L2832 S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 W2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886
K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 G2905 F2906 K2907 D2908 L2909 D2910 L2911 D2912 T2913 P2914 S2915 I2916 E2917 K2918 R2919 F2920 A2921 Y2922 S2923 F2924 L2925 Q2926 Q2927 L2928 I2929 R2930 Y2931 V2932 D2933 E2934 A2935 H2936 Q2937 Y2938 I2939 L2940 E2941 F2942 D2943 G2944 G2945 S2946
R2947 S2948 K2949 G2950 E2951 H2952 F2953 P2954 Y2955 E2956 Q2957 E2958 I2959 K2960 F2961 F2962 A2963 K2964 V2965 V2966 L2967 P2968 L2969 Q2972 Y2973 F2974 K2975 N2976 H2977 R2978 L2979 Y2980 F2981 L2982 S2983 A2984 A2985 S2986 R2987 P2988 L2989 C2990 T2991 G2992 G2993 H2994 A2995 S2996 N2997 K2998 E3001 L3006 F3007 C3008 K3009 L3010 G3011
V3012 L3013 H3016 R3017 I3018 S3019 L3020 P3021 G3022 N3023 D3024 A3025 T3026 S3027 I3028 V3029 N3030 C3031 L3032 H3033 I3034 L3035 G3036 Q3037 T3038 L3039 D3040 A3041 R3042 T3043 V3044 M3045 K3046 T3047 G3048 L3049 D3050 S3051 V3052 K3053 S3054 A3055 L3056 R3057 A3058 F3059 L3060 D3061 N3062 A3063 A3064 E3065 D3066 L3067 E3068 K3069 T3070 M3071 E3072
N3073 L3074 K3075 Q3076 G3077 Q3078 F3079 T3080 H3081 T3082 R3083 S3084 Q3085 P3086 K3087 G3088 V3089 T3090 Q3091 I3092 I3093 N3094 Y3095 T3096 T3097 V3098 A3099 L3100 L3101 P3102 M3103 L3104 S3105 S3106 L3107 F3108 E3109 H3110 I3111 G3112 Q3113 H3114 Q3115 F3116 G3117 E3118 D3119 L3120 I3121 L3122 E3123 D3124 V3125 Q3126 V3127 Y3130 R3131 I3132 L3133
T3134 S3135 L3136 Y3137 A3138 L3139 G3140 T3141 S3142 K3143 S3144 I3145 Y3146 V3147 E3148 R3149 Q3150 R3151 S3152 A3153 L3154 G3155 E3156 C3157 L3158 F3161 A3162 G3163 A3164 F3165 P3166 I3167 A3168 F3169 L3170 E3171 T3172 H3173 L3174 D3175 K3176 H3177 N3178 V3179 Y3180 S3181 I3182 Y3183 N3184 T3185 R3186 S3187 S3188 R3189 E3190 R3191 A3192 A3193 L3194
S3195 L3196 P3197 A3198 N3199 V3200 E3201 D3202 V3203 C3204 P3205 N3206 I3207 P3208 S3209 L3210 E3211 K3212 L3213 M3214 T3215 E3216 I3217 I3218 E3219 L3220 A3221 E3222 S3223 G3224 I3225 R3226 Y3227 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 Y3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 M3245 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253 E3254
N3255 H3256 P3257 E3258 R3259 A3260 E3261 M3262 C3263 C3264 T3265 A3266 L3267 N3268 S3269 E3270 H3271 M3272 N3273 T3274 L3275 L3276 G3277 N3278 I3279 L3280 K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 A3293 W3294 M3295 K3296 R3297 L3298 A3299 V3300 F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 L3314
K3315 T3316 H3317 F3318 L3319 P3320 L3321 M3322 E3323 K3324 L3325 K3326 K3327 K3328 A3329 A3330 M3331 V3332 V3333 S3334 E3335 E3336 D3337 H3338 L3339 K3340 A3341 E3342 A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 R3363 D3364 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374
F3375 V3376 D3377 Y3378 N3379 R3380 A3381 K3382 W3383 L3384 K3385 E3386 P3387 N3388 P3389 E3390 A3391 E3392 E3393 L3394 F3395 R3396 M3397 V3398 A3399 E3400 V3401 F3402 I3403 Y3404 W3405 S3406 K3407 S3408 HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR
LYS SER LYS MET SER LYS ALA ALA ILE SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG

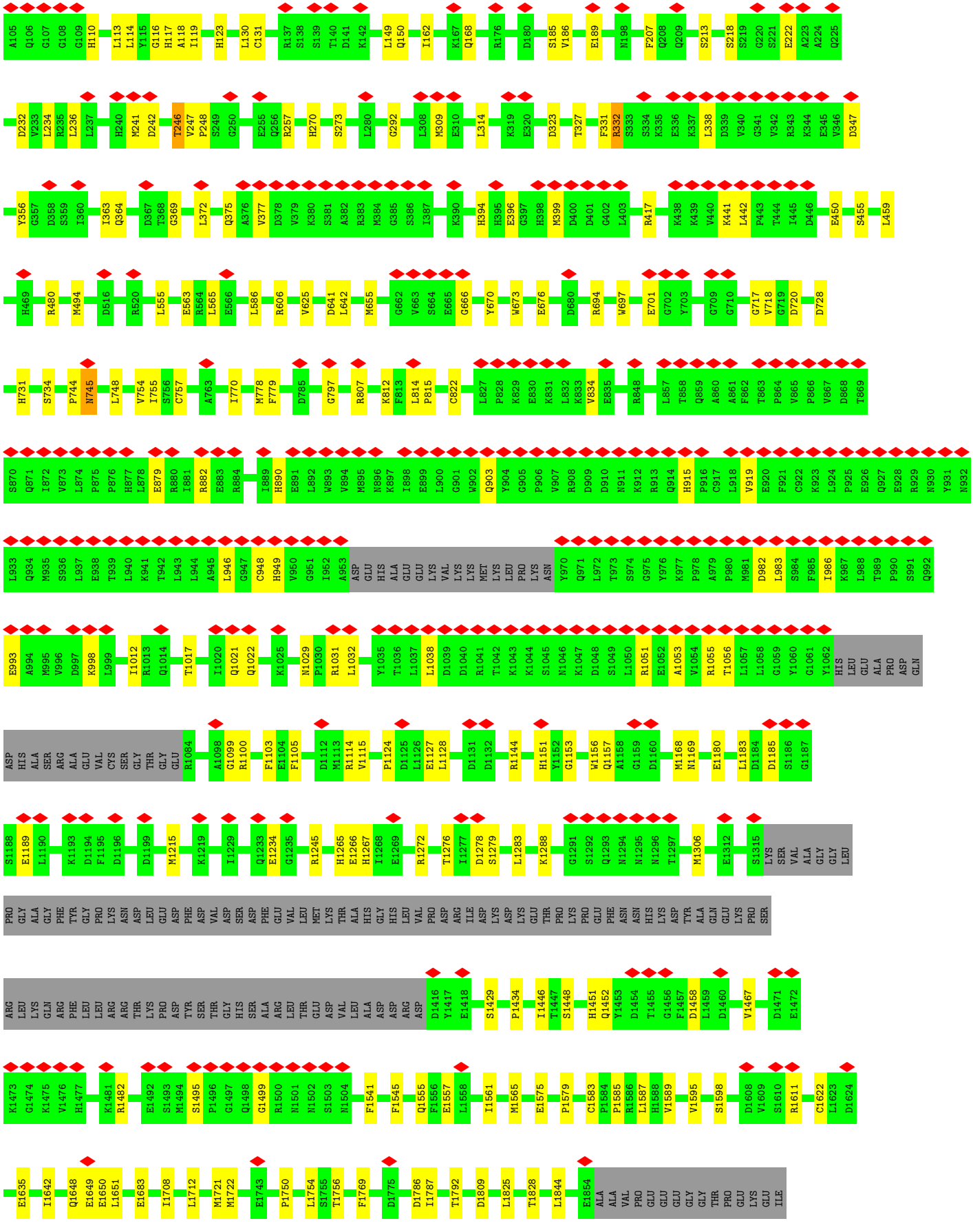


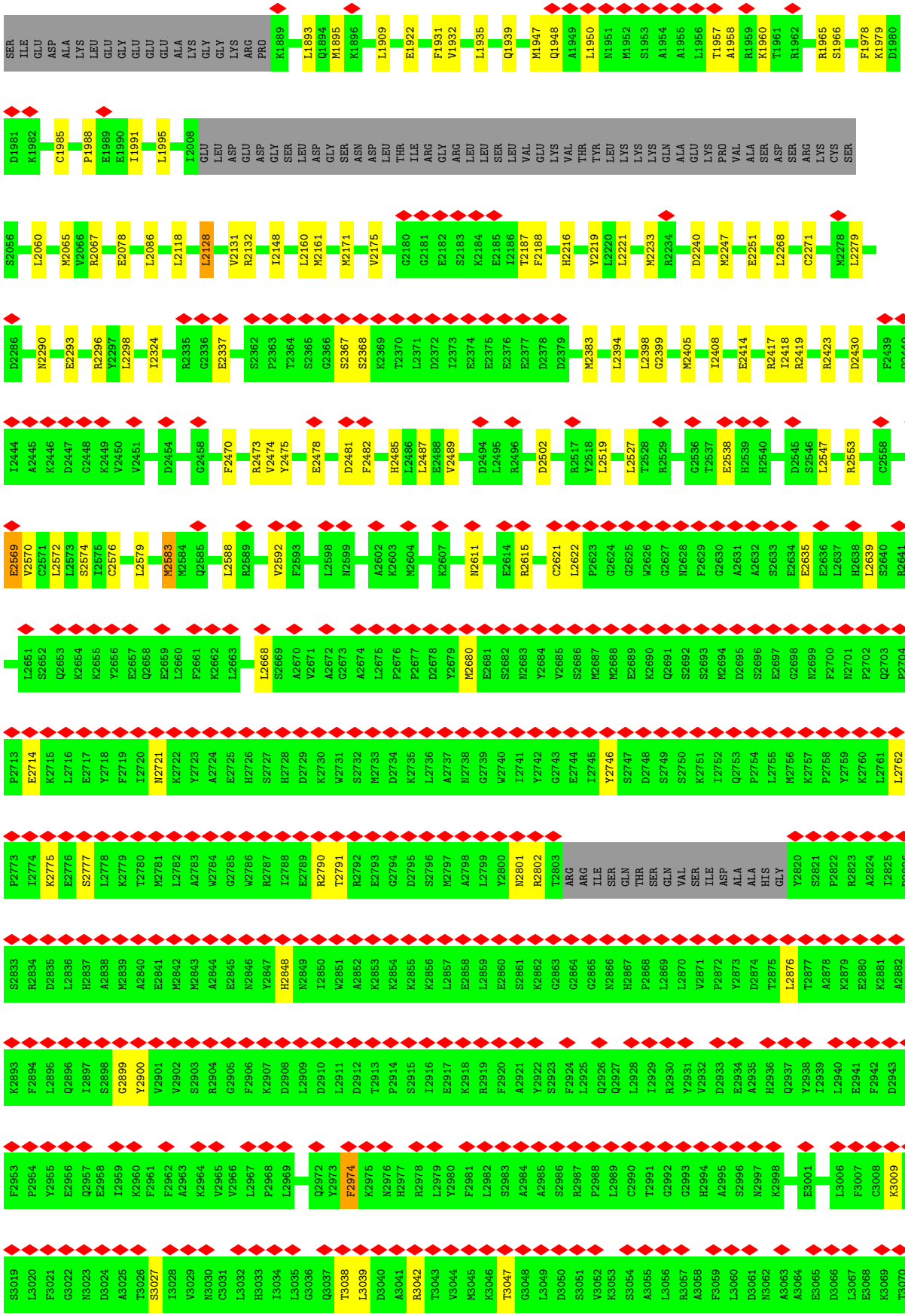
• Molecule 1: Ryanodine receptor 2

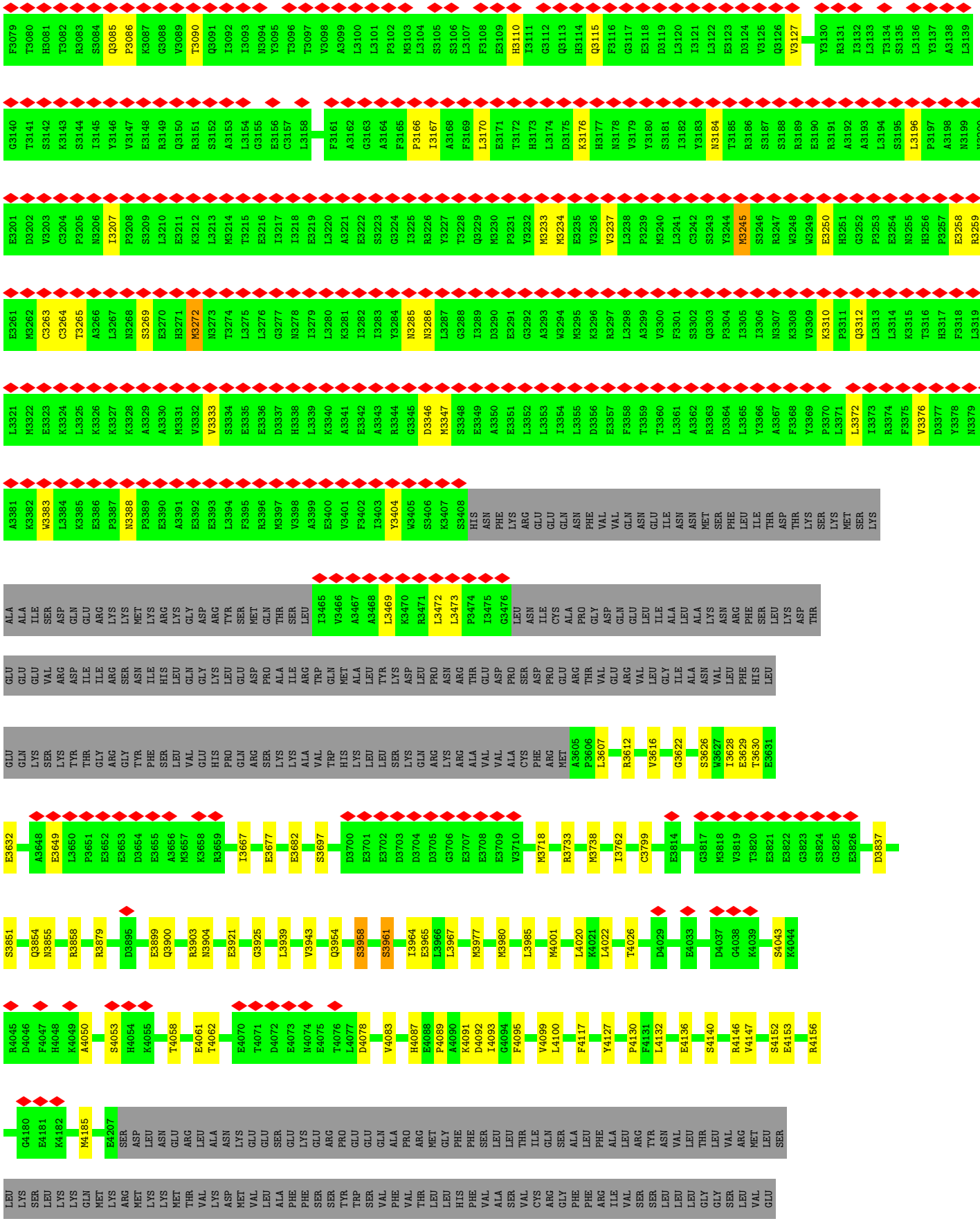
Chain B:

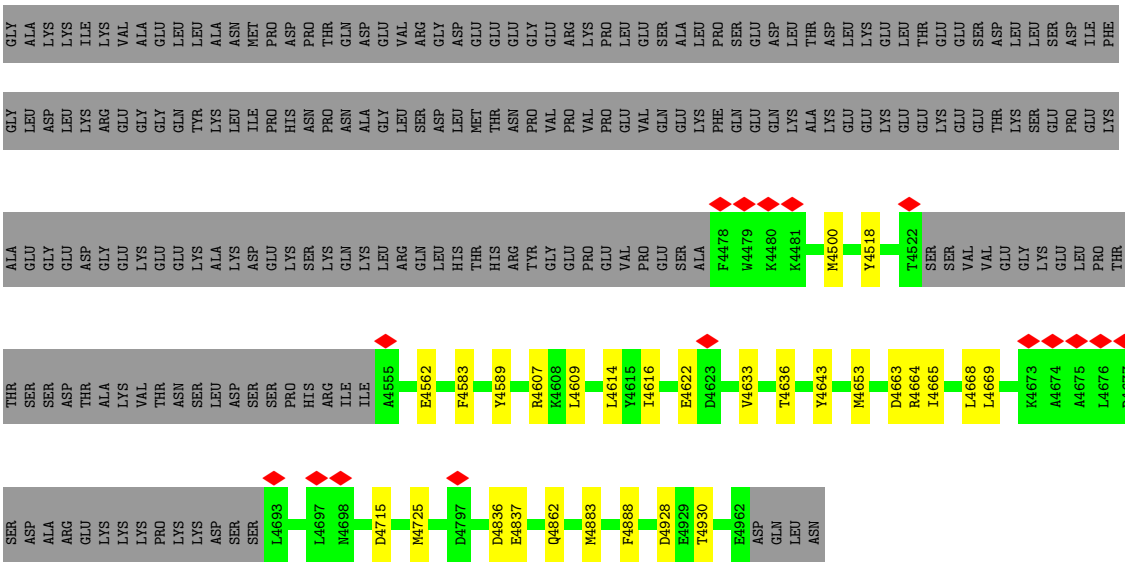





A105 Q106 G107 G108 G109 H110 L113 L114 Y115 G116 H117 A118 I119 H123 L130 C131 R137 S138 S139 T140 D141 K142 L149 Q150 I162 K167 Q168 R176 D180 S185 V186 E189 N198 F207 Q208 Q209 S213 S218 S219 G220 S221 E222 A223 A224 Q225
D232 Y233 L234 R235 L236 L237 H240 M241 D242 T246 V247 P248 S249 G250 E255 Q256 R257 H270 S273 L280 G292 L308 M309 E310 L314 K319 E320 D323 T327 F331 R332 S333 S334 K335 E336 K337 L338 D339 V340 G341 V342 R343 K344 E345 V346 D347
Y356 G357 D358 S359 I360 I363 Q364 D367 T368 G369 L372 Q375 A376 V377 D378 V379 K380 S381 A382 R383 M384 G385 S386 I387 K390 H394 H395 E396 G397 H398 M399 D400 D401 G402 L403 R417 K438 K439 V440 K441 L442 P443 T444 I445 D446 E450 S455 L459
H469 R480 M494 D516 R520 L555 E563 R564 L565 E566 L586 R606 V625 D641 L642 M655 G662 V663 S664 E665 G666 Y670 W673 E676 D680 R694 W697 E701 G702 Y703 G709 G710 G717 V718 G719 D720 D728
H731 S734 P744 N745 L748 V754 I755 S756 C757 A763 I770 M778 F779 D785 G797 R807 K812 F813 L814 P815 C822 L827 P828 K829 E830 K831 L832 K833 V834 E835 R848 L857 T858 Q859 A860 A861 F862 T863 P864 V865 P866 V867 D868 T869
S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 R884 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932
L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992
E993 A994 M995 V996 D997 K998 L999 I1012 R1013 Q1014 T1017 I1020 Q1021 Q1022 K1025 N1029 P1030 R1031 L1032 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS LEU GLU ALA PRO ASP GLN
ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 A1098 G1099 R1100 F1103 E1104 F1105 D1112 M1113 R1114 V1115 P1124 D1125 L1126 E1127 L1128 D1131 D1132 R1144 H1151 Y1152 G1153 W1156 Q1157 A1158 G1159 D1160 M1168 N1169 E1180 L1183 D1184 D1185 S1186 G1187
S1188 E1189 L1190 K1193 D1194 F1195 D1196 D1199 M1215 K1219 I1229 Q1233 E1234 G1235 R1245 H1265 E1266 H1267 I1268 E1269 R1272 T1276 I1277 D1278 S1279 L1283 K1288 G1291 S1292 Q1293 N1294 N1295 N1296 T1297 M1306 E1312 S1315 LYS SER VAL ALA GLY GLY LEU
PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER
ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1417 E1418 S1429 P1434 I1446 T1447 S1448 H1451 Q1452 Y1453 D1454 T1455 G1456 F1457 D1458 L1459 D1460 V1467 D1471 E1472
K1473 G1474 K1475 V1476 H1477 K1481 R1482 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 S1503 N1504 F1541 F1545 Q1555 F1556 E1557 L1558 I1561 M1565 E1575 P1579 C1583 P1584 P1585 R1586 L1587 H1588 V1589 V1595 S1598 D1608 V1609 S1610 R1611 C1622 L1623 D1624
E1635 I1642 Q1648 E1649 E1650 L1651 E1683 I1708 L1712 M1721 M1722 E1743 P1750 L1754 S1755 T1756 F1769 D1775 D1786 I1787 T1792 D1809 L1825 T1828 L1844 E1854 ALA ALA VAL PRO GLU GLU GLY GLY THR PRO GLU LYS GLU ILE


SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 L1893 Q1894 M1895 K1896 L1909 E1922 F1931 V1932 L1935 Q1939 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 R1965 S1966 F1978 K1979 D1980
D1981 K1982 C1985 P1988 E1989 E1990 I1991 L1995 I2008 GLU LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA ALA SER ASP SER ARG LYS CYS SER
S2056 L2060 M2065 V2066 R2067 E2078 L2086 L2118 L2128 V2131 R2132 I2148 L2160 M2161 M2171 V2175 G2180 G2181 E2182 S2183 K2184 E2185 I2186 T2187 F2188 H2216 Y2219 L2220 L2221 M2233 R2234 D2240 M2247 E2251 L2268 C2271 M2278 L2279
D2286 N2290 E2293 R2296 Y2297 L2298 I2324 R2335 G2336 E2337 S2362 P2363 T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 M2383 L2394 L2398 G2399 M2405 I2408 E2414 R2417 I2418 R2419 R2423 D2430 F2439 Q2440 T2443
I2444 A2445 K2446 D2447 G2448 K2449 V2450 V2451 D2454 G2458 F2470 R2473 V2474 Y2475 E2478 D2481 F2482 H2485 L2486 L2487 E2488 V2489 D2494 L2495 R2496 D2502 R2517 Y2518 L2519 L2527 T2528 R2529 G2536 T2537 E2538 H2539 H2540 D2545 S2546 L2547 R2553 C2558 R2565
E2569 V2570 C2571 L2572 L2573 S2574 I2575 C2576 L2579 M2583 M2584 Q2585 L2588 R2589 V2592 F2593 L2598 N2599 A2602 K2603 M2604 K2607 N2611 E2614 R2615 C2621 L2622 P2623 G2624 G2625 W2626 G2627 N2628 F2629 G2630 A2631 A2632 S2633 E2634 E2635 E2636 L2637 H2638 L2639 S2640 R2641 K2642 L2643 P2644 W2645
L2651 S2652 Q2653 K2654 K2655 Y2656 E2657 Q2658 E2659 L2660 F2661 K2662 L2663 L2668 S2669 A2670 V2671 A2672 G2673 A2674 L2675 P2676 P2677 D2678 Y2679 M2680 E2681 S2682 N2683 Y2684 V2685 S2686 M2687 M2688 E2689 K2690 Q2691 S2692 S2693 M2694 D2695 S2696 E2697 G2698 N2699 P2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707 S2708 N2709 I2710 T2711 I2712
P2713 E2714 K2715 L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772
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S2833 R2834 D2835 L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 D2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892
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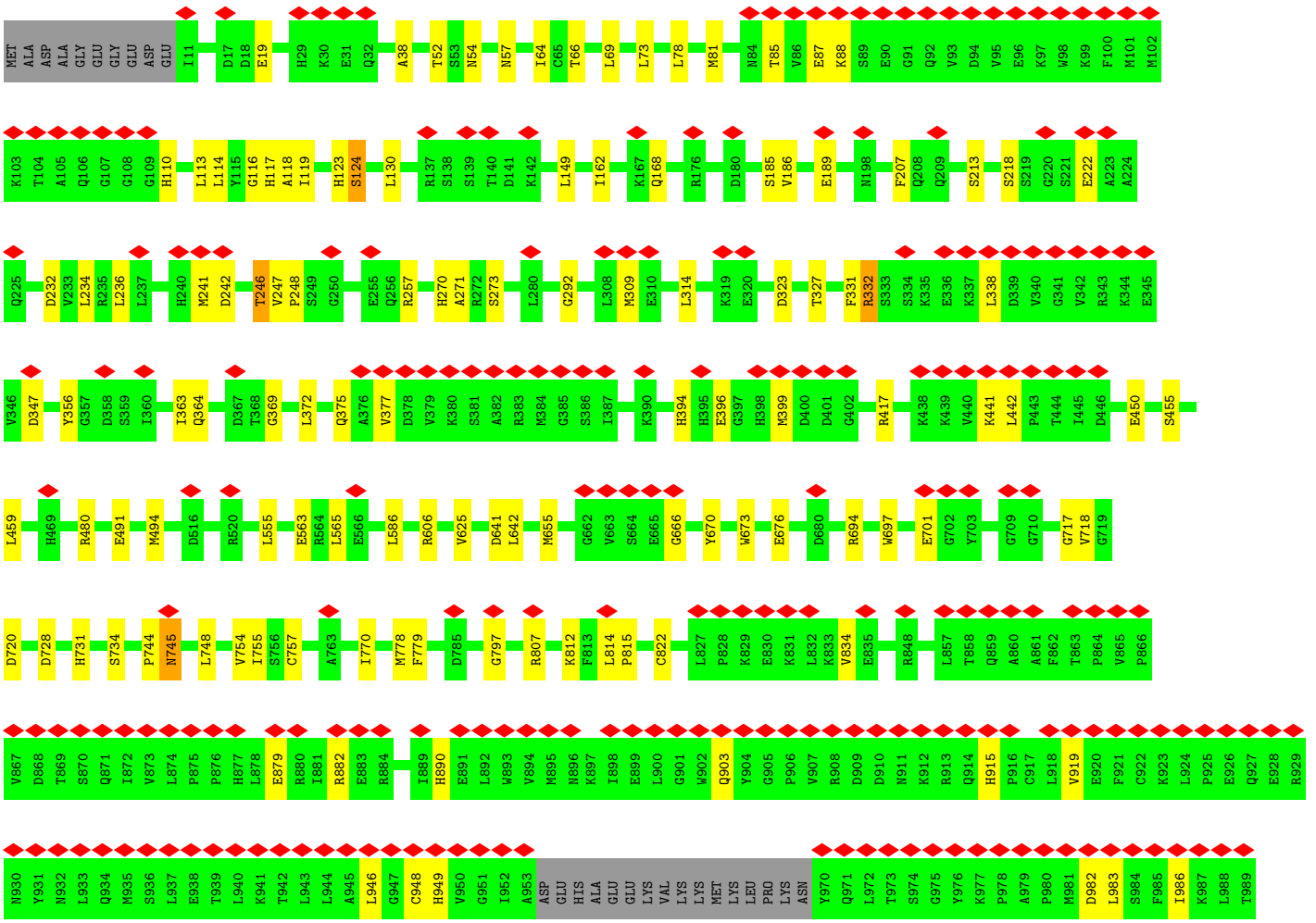

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ALA ALA ILE SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR
GLU GLU GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO SER ASP PRO GLU GLN ARG THR VAL GLU ARG VAL LEU GLY ILE ALA ASN VAL LEU GLY PHE HIS LEU
GLU GLN LYS SER LYS TYR THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET A3605 P3606 L3607 R3612 V3616 G3622 S3626 W3627 I3628 E3629 T3630 E3631
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R4045 D4046 F4047 H4048 K4049 A4050 S4053 H4054 K4055 T4058 E4061 T4062 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077 D4078 V4083 H4087 E4088 P4089 A4090 K4091 D4092 I4093 G4094 F4095 V4099 L4100 F4117 Y4127 P4130 F4131 L4132 E4136 S4140 R4146 V4147 S4152 E4153 R4156
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LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU VAL GLU

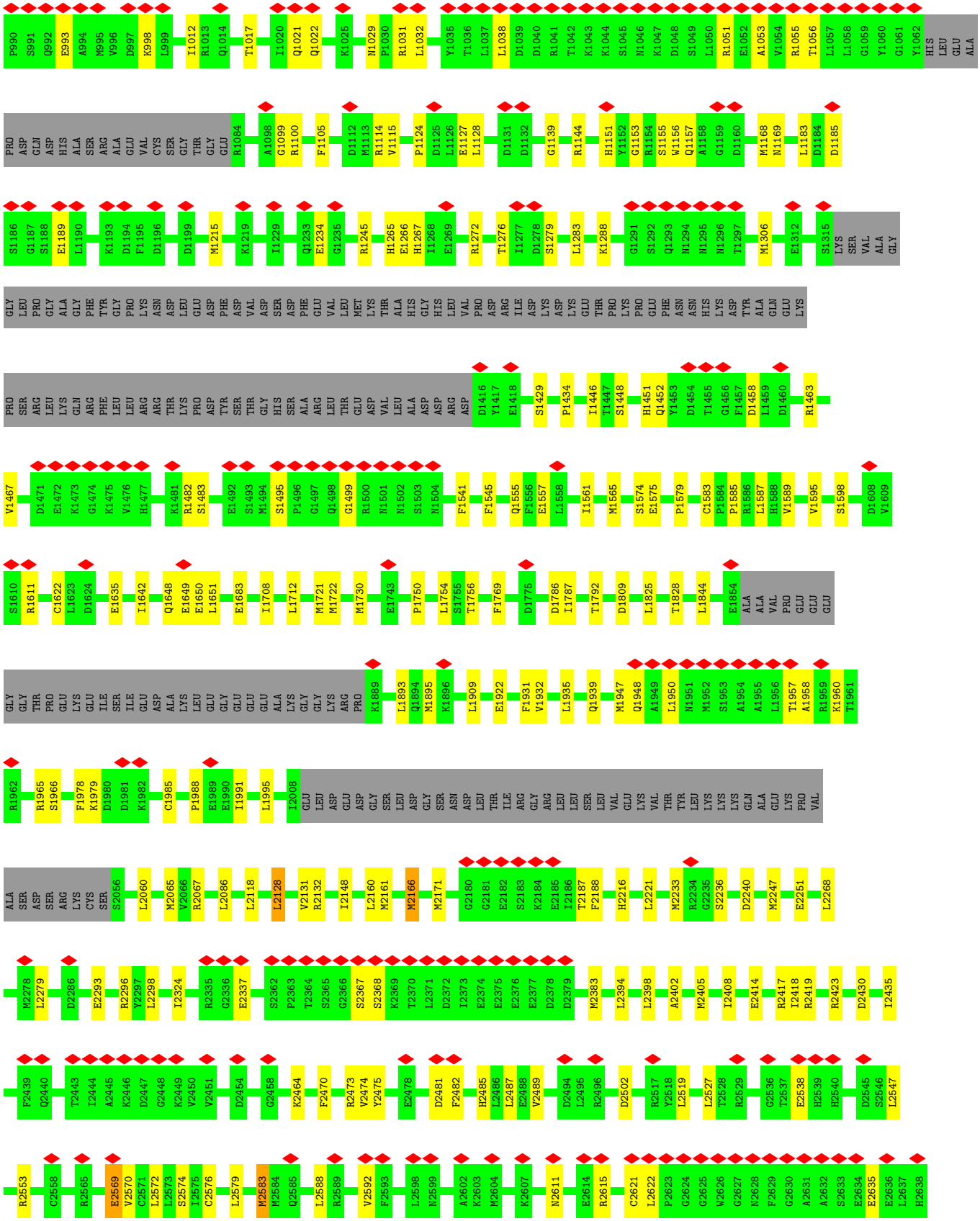


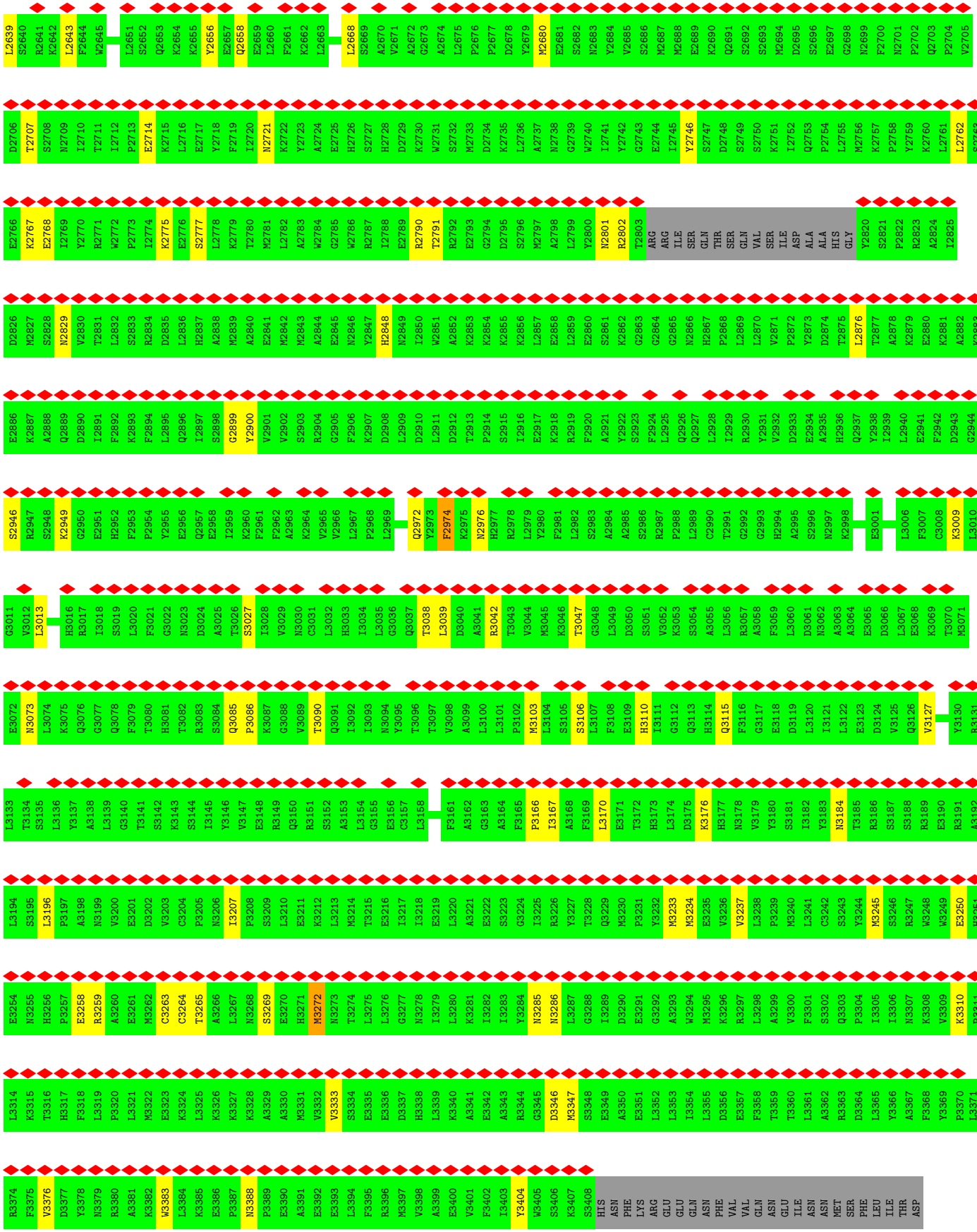
• Molecule 1: Ryanodine receptor 2

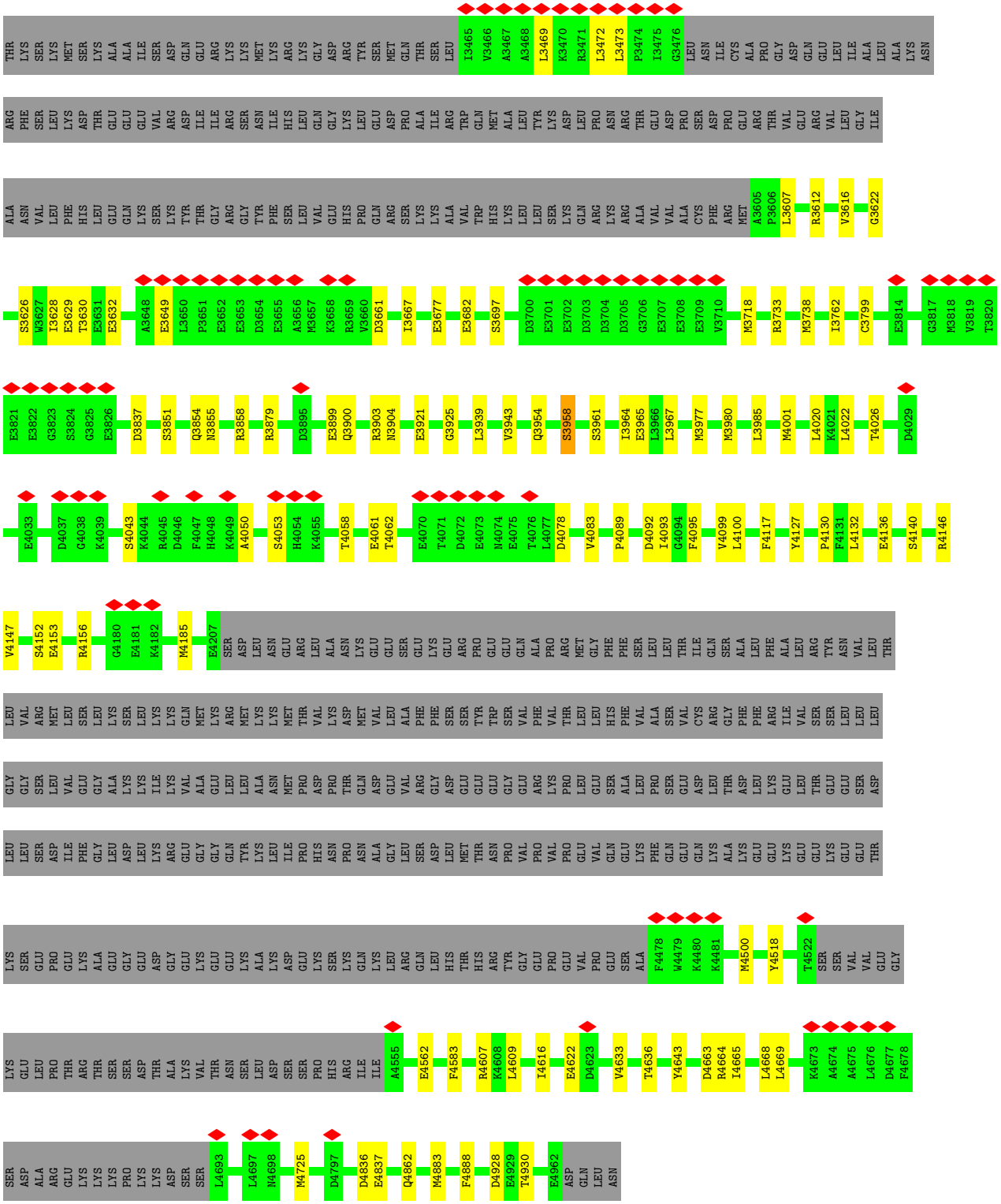
Chain C:






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PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 A1098 G1099 R1100 F1105 D1112 M1113 R1114 V1115 P1124 D1125 L1126 E1127 L1128 D1131 D1132 G1139 R1144 H1151 Y1152 G1153 R1154 S1155 W1156 Q1157 A1158 G1159 D1160 M1168 N1169 L1183 D1184 D1185
S1186 G1187 S1188 E1189 L1190 K1193 D1194 F1195 D1196 D1199 M1215 K1219 I1229 Q1233 E1234 G1235 R1245 H1265 E1266 H1267 I1268 E1269 R1272 T1276 I1277 D1278 S1279 L1283 K1288 G1291 S1292 Q1293 N1294 N1295 N1296 T1297 M1306 E1312 S1315 LYS SER VAL ALA GLY
GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS
PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1417 E1418 S1429 P1434 I1446 T1447 S1448 H1451 Q1452 Y1453 D1454 T1455 G1456 F1457 D1458 L1459 D1460 R1463
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GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 L1893 Q1894 M1895 K1896 L1909 E1922 F1931 V1932 L1935 Q1939 M1947 Q1948 A1949 L1950 N1951 M1962 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961
R1962 R1965 S1966 F1978 K1979 D1980 D1981 K1982 C1985 P1988 E1989 E1990 I1991 L1995 I2008 GLU LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL
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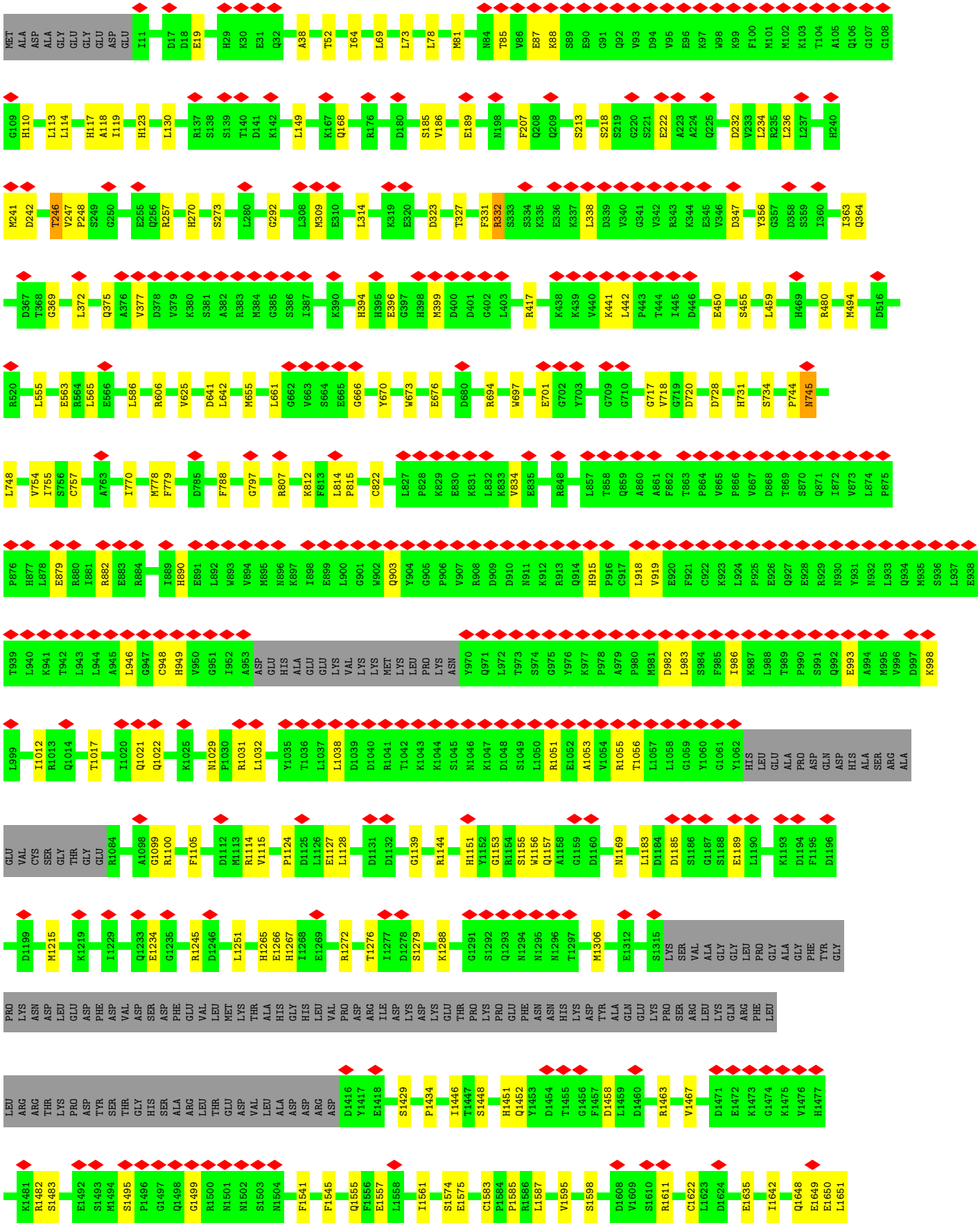

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D2826 M2827 S2828 N2829 V2830 D2890 I2891 F2892 K2893 F2894 L2895 Q2896 I2897 S2898 G2899 Y2900 V2901 V2902 S2903 R2904 G2905 F2906 K2907 D2908 L2909 D2910 L2911 D2912 T2913 P2914 S2915 I2916 E2917 K2918 R2919 F2920 A2921 Y2922 S2923 F2924 L2925 Q2926 Q2927 L2928 I2929 R2930 Y2931 V2932 D2933 E2934 A2935 H2936 Q2937 Y2938 I2939 L2940 E2941 F2942 D2943 G2944 G2945
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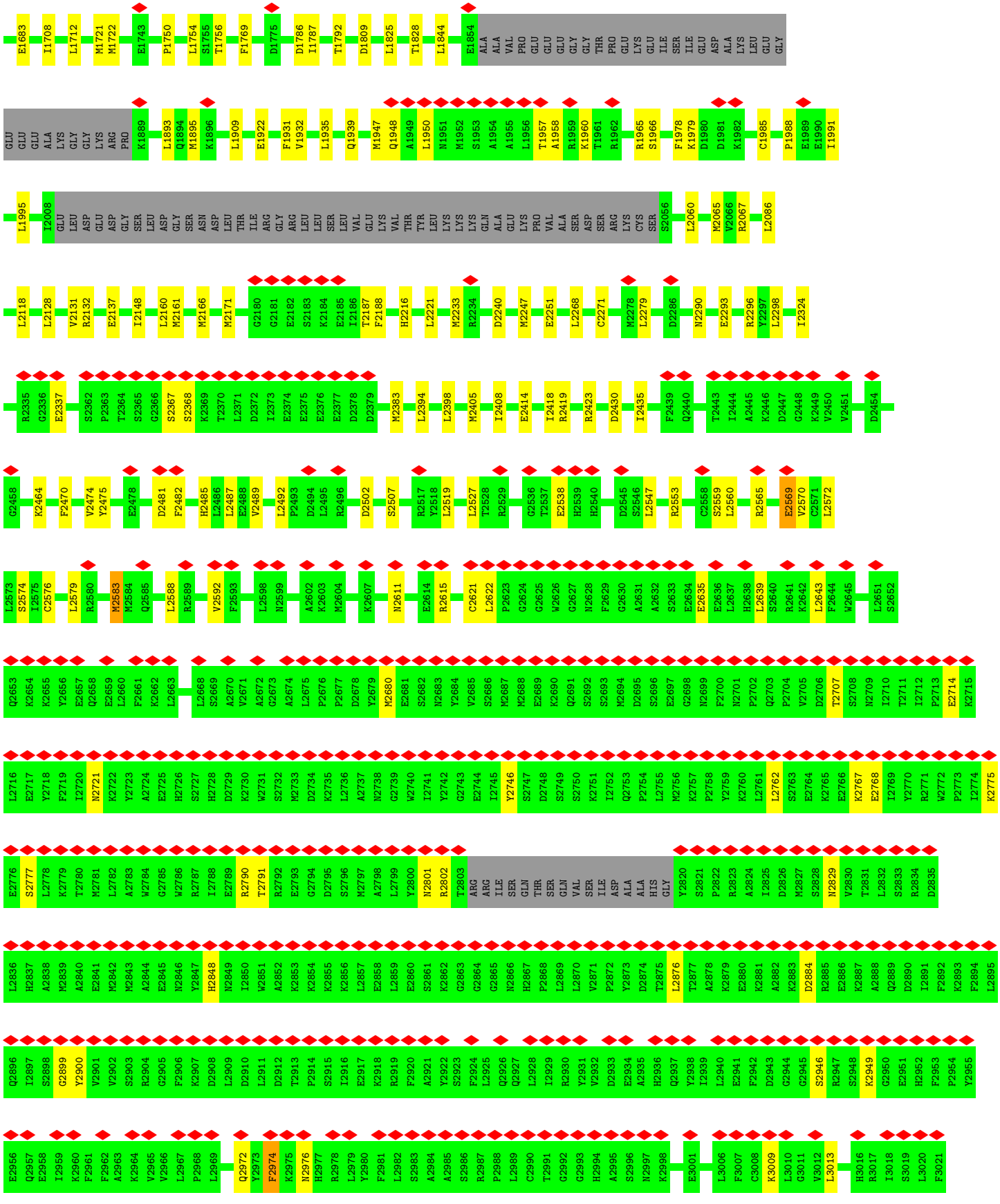


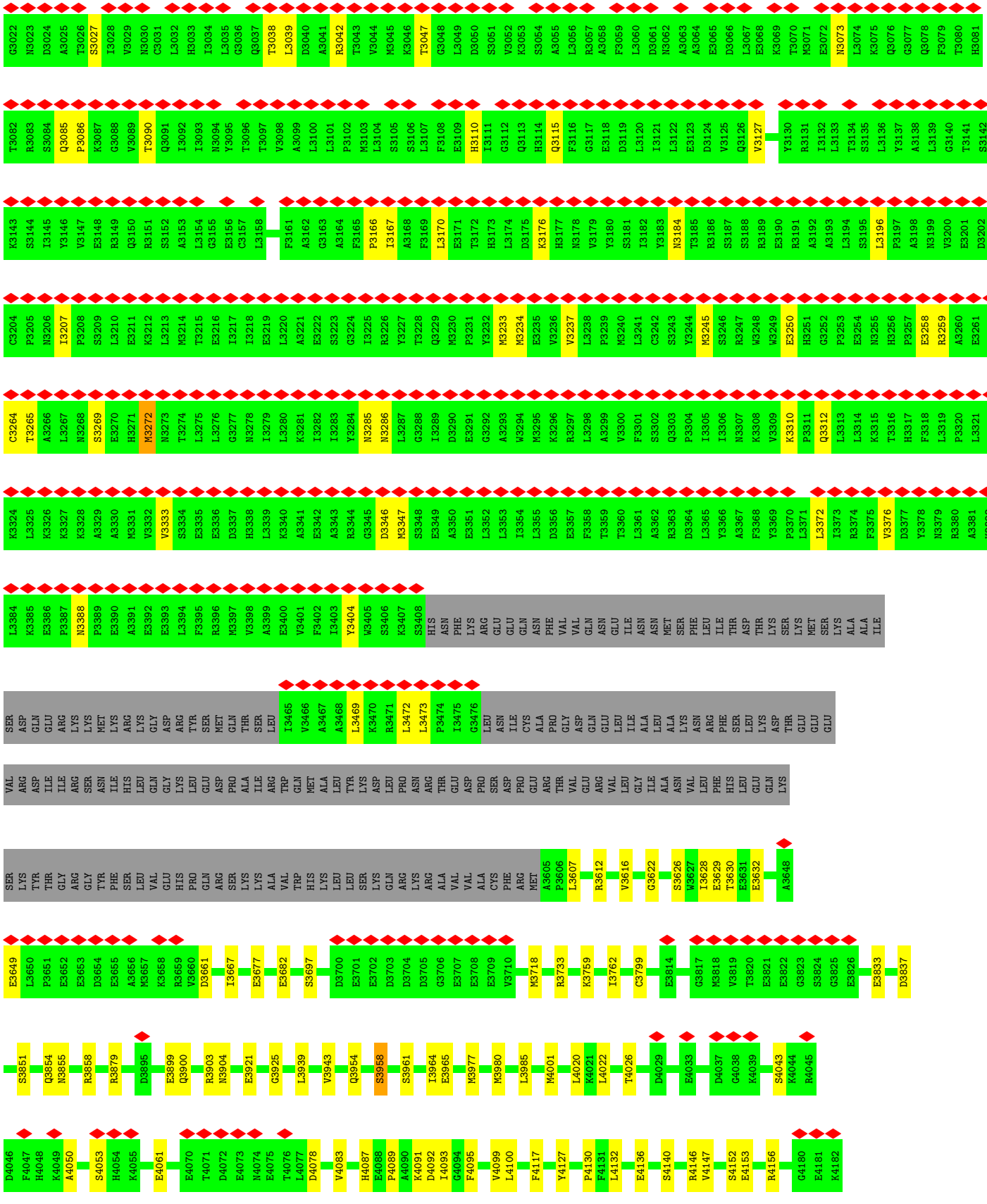
• Molecule 1: Ryanodine receptor 2

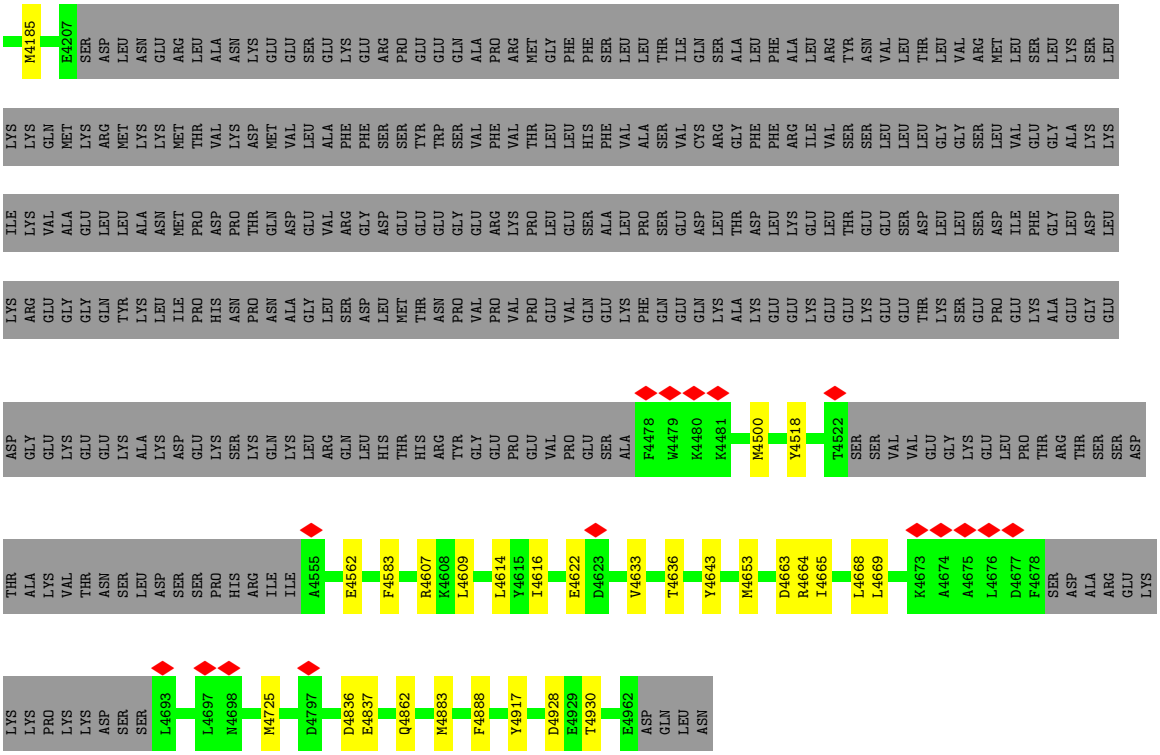
Chain D:




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M241 D242 T246 V247 P248 S249 G250 E255 Q256 R257 H270 S273 L280 G292 L308 M309 E310 L314 K319 E320 D323 T327 F331 R332 S333 S334 K335 E336 K337 L338 D339 V340 G341 V342 R343 K344 E345 V346 D347 Y356 G357 D358 S359 I360 I363 Q364
D367 T368 G369 L372 Q375 A376 V377 D378 V379 K380 S381 A382 R383 M384 G385 S386 I387 K390 H394 H395 E396 G397 H398 M399 D400 D401 G402 L403 R417 K438 K439 V440 K441 L442 P443 T444 I445 D446 E450 S455 L459 H469 R480 M494 D516
R520 L555 E563 R564 L565 E566 L586 R606 V625 D641 L642 M655 L661 G662 V663 S664 E665 G666 Y670 W673 E676 D680 R694 W697 E701 G702 Y703 G709 G710 G717 V718 G719 D720 D728 H731 S734 P744 N745
L748 V754 I755 S756 C757 A763 I770 M778 F779 D785 F788 G797 R807 K812 F813 L814 P815 C822 L827 P828 K829 E830 K831 L832 K833 V834 E835 R848 L857 T858 Q859 A860 A861 F862 T863 P864 V865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875
P876 H877 L878 E879 R880 I881 R882 E883 R884 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 C922 K923 L924 P925 E926 Q927 E928 R929 N930 Y931 N932 L933 Q934 M935 S936 L937 E938
T939 L940 K941 T942 L943 L944 A945 L946 G947 C948 H949 V950 G951 I952 A953 ASP GLU HIS ALA GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 D997 K998
L999 I1012 R1013 Q1014 T1017 I1020 Q1021 Q1022 K1025 N1029 P1030 R1031 L1032 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA
GLU VAL CYS SER GLY THR GLY GLU R1084 A1098 G1099 R1100 F1105 D1112 M1113 R1114 V1115 P1124 D1125 L1126 E1127 L1128 D1131 D1132 G1139 R1144 H1151 Y1152 G1153 R1154 S1155 W1156 Q1157 A1158 G1159 D1160 N1169 L1183 D1184 D1185 S1186 G1187 S1188 E1189 L1190 K1193 D1194 F1195 D1196
D1199 M1215 K1219 I1229 Q1233 E1234 G1235 R1245 D1246 L1251 H1265 E1266 H1267 I1268 E1269 R1272 T1276 I1277 D1278 S1279 K1288 G1291 S1292 Q1293 N1294 N1295 N1296 T1297 M1306 E1312 S1315 LYS SER VAL ALA GLY GLY LEU PRO GLY ALA GLY PHE TYR GLY
PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU
LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP D1416 Y1417 E1418 S1429 P1434 I1446 T1447 S1448 H1451 Q1452 Y1453 D1454 T1455 G1456 F1457 D1458 L1459 D1460 R1463 V1467 D1471 E1472 K1473 G1474 K1475 V1476 H1477
K1481 R1482 S1483 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 S1503 N1504 F1541 F1545 Q1555 F1556 E1557 L1558 I1561 S1574 E1575 C1583 P1584 P1585 R1586 L1587 V1595 S1598 D1608 V1609 S1610 R1611 C1622 L1623 D1624 E1635 I1642 Q1648 E1649 E1650 L1651


E1683 I1708 L1712 M1721 M1722 E1743 P1750 L1754 S1755 T1756 F1769 D1775 D1786 I1787 T1792 D1809 L1825 T1828 L1844 E1854 ALA ALA VAL PRO GLU GLU GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY
GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO K1889 L1893 Q1894 M1895 K1896 L1909 E1922 F1931 V1932 L1935 Q1939 M1947 Q1948 A1949 L1950 N1951 M1952 S1953 A1954 A1955 L1956 T1957 A1958 R1959 K1960 T1961 R1962 R1965 S1966 F1978 K1979 D1980 D1981 K1982 C1985 P1988 E1989 E1990 I1991
L1995 I2008 GLU LEU ASP GLU ASP GLY SER LEU ASP GLY SER ASN ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER S2056 L2060 M2065 V2066 R2067 L2086
L2118 L2128 V2131 R2132 E2137 I2148 L2160 M2161 M2166 M2171 G2180 G2181 E2182 S2183 K2184 E2185 I2186 T2187 F2188 H2216 L2221 M2233 R2234 D2240 M2247 E2251 L2268 C2271 M2278 L2279 D2286 N2290 E2293 R2296 Y2297 L2298 I2324
R2335 G2336 E2337 S2362 P2363 T2364 S2365 G2366 S2367 S2368 K2369 T2370 L2371 D2372 I2373 E2374 E2375 E2376 E2377 D2378 D2379 M2383 L2394 L2398 M2405 I2408 E2414 I2418 R2419 R2423 D2430 I2435 F2439 Q2440 T2443 I2444 A2445 K2446 D2447 G2448 K2449 V2450 V2451 D2454
G2458 K2464 F2470 V2474 Y2475 E2478 D2481 F2482 H2485 L2486 L2487 E2488 V2489 L2492 P2493 D2494 L2495 R2496 D2502 S2507 R2517 Y2518 L2519 L2527 T2528 R2529 G2536 T2537 E2538 H2539 H2540 D2545 S2546 L2547 R2553 C2558 S2559 L2560 R2565 E2569 V2570 C2571 L2572
L2573 S2574 I2575 C2576 L2579 R2580 M2583 M2584 Q2585 L2588 R2589 V2592 F2593 L2598 N2599 A2602 K2603 M2604 K2607 N2611 E2614 R2615 C2621 L2622 P2623 G2624 G2625 W2626 G2627 N2628 F2629 G2630 A2631 A2632 S2633 E2634 E2635 E2636 L2637 H2638 L2639 S2640 R2641 K2642 L2643 F2644 W2645 L2651 S2652
Q2653 K2654 K2655 Y2656 E2657 Q2658 E2659 L2660 F2661 K2662 L2663 L2668 S2669 A2670 V2671 A2672 G2673 A2674 L2675 P2676 P2677 D2678 Y2679 M2680 E2681 S2682 N2683 Y2684 V2685 S2686 M2687 M2688 E2689 K2690 Q2691 S2692 S2693 M2694 D2695 S2696 E2697 G2698 N2699 F2700 N2701 P2702 Q2703 P2704 V2705 D2706 T2707 S2708 N2709 I2710 T2711 I2712 P2713 E2714 K2715
L2716 E2717 Y2718 F2719 I2720 N2721 K2722 Y2723 A2724 E2725 H2726 S2727 H2728 D2729 K2730 W2731 S2732 M2733 D2734 K2735 L2736 A2737 N2738 G2739 W2740 I2741 Y2742 G2743 E2744 I2745 Y2746 S2747 D2748 S2749 S2750 K2751 I2752 Q2753 P2754 L2755 M2756 K2757 P2758 Y2759 K2760 L2761 L2762 S2763 E2764 K2765 E2766 K2767 E2768 I2769 Y2770 R2771 W2772 P2773 I2774 K2775
E2776 S2777 L2778 K2779 T2780 M2781 L2782 A2783 W2784 G2785 W2786 R2787 I2788 E2789 R2790 T2791 R2792 E2793 G2794 D2795 S2796 M2797 A2798 L2799 Y2800 N2801 R2802 T2803 ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY Y2820 S2821 P2822 R2823 A2824 I2825 L2826 M2827 S2828 N2829 V2830 T2831 L2832 S2833 R2834 D2835
L2836 H2837 A2838 M2839 A2840 E2841 M2842 M2843 A2844 E2845 N2846 Y2847 H2848 N2849 I2850 W2851 A2852 K2853 K2854 K2855 K2856 L2857 E2858 L2859 E2860 S2861 K2862 G2863 G2864 G2865 N2866 H2867 P2868 L2869 L2870 V2871 P2872 Y2873 A2874 T2875 L2876 T2877 A2878 K2879 E2880 K2881 A2882 K2883 D2884 R2885 E2886 K2887 A2888 Q2889 D2890 I2891 F2892 K2893 F2894 L2895
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E2956 Q2957 E2958 I2959 K2960 F2961 F2962 A2963 K2964 V2965 V2966 L2967 P2968 L2969 Q2972 Y2973 F2974 K2975 N2976 H2977 R2978 L2979 Y2980 F2981 L2982 S2983 A2984 A2985 S2986 R2987 P2988 L2989 C2990 T2991 G2992 G2993 H2994 A2995 S2996 N2997 K2998 E3001 L3006 F3007 C3008 K3009 L3010 G3011 V3012 L3013 H3016 R3017 I3018 S3019 L3020 F3021

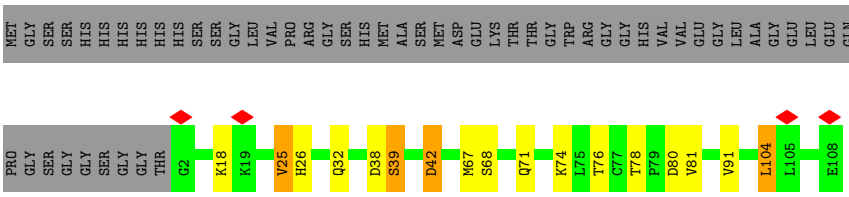

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T3082 R3083 S3084 Q3085 P3086 K3087 G3088 V3089 T3090 Q3091 I3092 I3093 N3094 Y3095 T3096 T3097 V3098 A3099 L3100 L3101 P3102 M3103 L3104 S3105 S3106 L3107 F3108 E3109 H3110 I3111 G3112 Q3113 H3114 Q3115 F3116 G3117 E3118 D3119 L3120 I3121 L3122 E3123 D3124 V3125 Q3126 V3127 Y3130 R3131 I3132 L3133 T3134 S3135 L3136 Y3137 A3138 L3139 G3140 T3141 S3142
K3143 S3144 I3145 Y3146 V3147 E3148 R3149 Q3150 R3151 S3152 A3153 L3154 G3155 E3156 C3157 L3158 F3161 A3162 G3163 A3164 F3165 P3166 I3167 A3168 F3169 L3170 E3171 T3172 H3173 L3174 D3175 K3176 H3177 N3178 V3179 Y3180 S3181 I3182 Y3183 N3184 T3185 R3186 S3187 S3188 R3189 E3190 R3191 A3192 A3193 L3194 S3195 L3196 P3197 A3198 N3199 V3200 E3201 D3202 V3203
C3204 P3205 N3206 I3207 P3208 S3209 L3210 E3211 K3212 L3213 M3214 T3215 E3216 I3217 I3218 E3219 L3220 A3221 E3222 S3223 G3224 I3225 R3226 Y3227 T3228 Q3229 M3230 P3231 Y3232 M3233 M3234 E3235 V3236 V3237 L3238 P3239 M3240 L3241 C3242 S3243 Y3244 M3245 S3246 R3247 W3248 W3249 E3250 H3251 G3252 P3253 E3254 N3255 H3256 P3257 E3258 R3259 A3260 E3261 M3262 C3263
C3264 T3265 A3266 L3267 N3268 S3269 E3270 H3271 M3272 N3273 T3274 L3275 L3276 G3277 N3278 I3279 L3280 K3281 I3282 I3283 Y3284 N3285 N3286 L3287 G3288 I3289 D3290 E3291 G3292 A3293 W3294 M3295 K3296 R3297 L3298 A3299 V3300 F3301 S3302 Q3303 P3304 I3305 I3306 N3307 K3308 V3309 K3310 P3311 Q3312 L3313 L3314 K3315 T3316 H3317 F3318 L3319 P3320 L3321 M3322 E3323
K3324 L3325 K3326 K3327 K3328 A3329 A3330 M3331 V3332 V3333 S3334 E3335 E3336 D3337 H3338 L3339 K3340 A3341 E3342 A3343 R3344 G3345 D3346 M3347 S3348 E3349 A3350 E3351 L3352 L3353 I3354 L3355 D3356 E3357 F3358 T3359 T3360 L3361 A3362 R3363 D3364 L3365 Y3366 A3367 F3368 Y3369 P3370 L3371 L3372 I3373 R3374 F3375 V3376 D3377 Y3378 N3379 R3380 A3381 K3382 W3383
L3384 K3385 E3386 P3387 N3388 P3389 E3390 A3391 E3392 E3393 L3394 F3395 R3396 M3397 V3398 A3399 E3400 V3401 F3402 I3403 Y3404 W3405 S3406 K3407 S3408 HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA ILE
SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU I3465 V3466 A3467 A3468 L3469 K3470 R3471 L3472 L3473 P3474 I3475 G3476 LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU GLU
VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP PRO SER ASP PRO GLU ARG THR VAL GLU ARG VAL LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU LEU LYS
SER LYS TYR THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA CYS PHE ARG MET A3605 P3606 L3607 R3612 V3616 G3622 S3626 W3627 I3628 E3629 T3630 E3631 E3632 A3648
E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 V3660 D3661 I3667 E3677 E3682 S3697 D3700 E3701 E3702 D3703 D3704 D3705 G3706 E3707 E3708 E3709 V3710 M3718 R3733 K3759 I3762 C3799 E3814 G3817 M3818 Y3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 E3833 D3837
S3851 Q3854 N3855 R3858 R3879 D3895 E3899 Q3900 R3903 N3904 E3921 G3925 L3939 V3943 Q3954 S3958 S3961 I3964 E3965 M3977 M3980 L3985 M4001 L4020 K4021 L4022 T4026 D4029 E4033 D4037 G4038 K4039 S4043 K4044 R4045
D4046 F4047 H4048 K4049 A4050 S4053 H4054 K4055 E4061 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077 D4078 V4083 H4087 E4088 P4089 A4090 K4091 D4092 I4093 G4094 F4095 V4099 L4100 F4117 Y4127 P4130 F4131 L4132 E4136 S4140 R4146 V4147 S4152 E4153 R4156 G4180 E4181 K4182



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

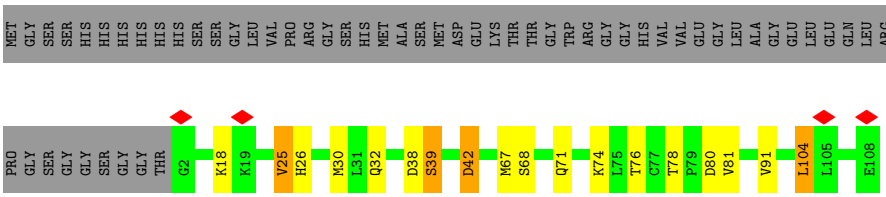




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



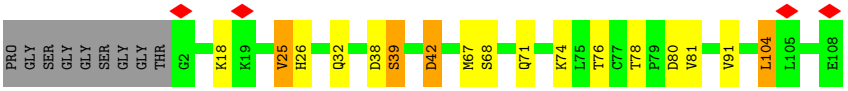


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

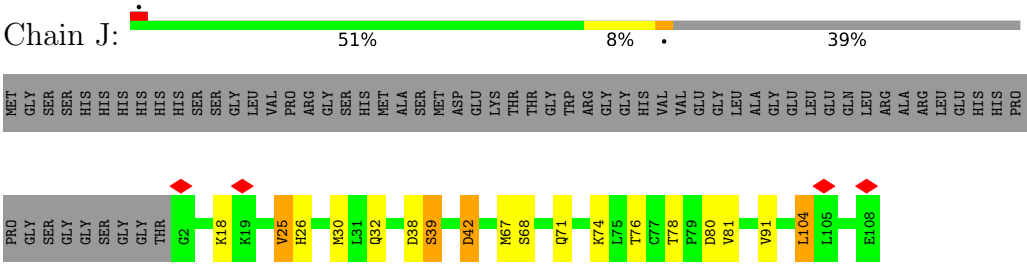
Chain I:







• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	45610	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	469.504, 469.504, 469.504	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.917, 0.917, 0.917	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.19	0/34495	0.43	0/46614
1	B	0.19	0/34495	0.43	0/46614
1	C	0.19	0/34495	0.43	0/46614
1	D	0.19	0/34495	0.43	0/46614
2	G	0.22	0/835	0.51	0/1123
2	H	0.22	0/835	0.49	0/1123
2	I	0.22	0/835	0.51	0/1123
2	J	0.22	0/835	0.51	0/1123
All	All	0.19	0/141320	0.43	0/190948

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3925	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	3925	GLY	Peptide
1	C	3925	GLY	Peptide
1	D	3925	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33753	33380	33379	288	0
1	B	33753	33380	33379	285	0
1	C	33753	33380	33379	287	0
1	D	33753	33380	33379	282	0
2	G	819	821	821	10	0
2	H	819	821	821	10	0
2	I	819	821	821	10	0
2	J	819	821	821	10	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	138292	136804	136800	1164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3954:GLN:O	1:D:3958:SER:OG	2.04	0.76
1:C:3954:GLN:O	1:C:3958:SER:OG	2.04	0.75
1:B:3622:GLY:O	1:B:3626:SER:OG	2.03	0.74
1:A:3954:GLN:O	1:A:3958:SER:OG	2.04	0.74
1:B:3954:GLN:O	1:B:3958:SER:OG	2.04	0.73
1:C:3622:GLY:O	1:C:3626:SER:OG	2.03	0.72
1:A:3855:ASN:OD1	1:A:3858:ARG:NH2	2.23	0.72
1:B:3855:ASN:OD1	1:B:3858:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3855:ASN:OD1	1:D:3858:ARG:NH2	2.23	0.72
1:D:3622:GLY:O	1:D:3626:SER:OG	2.03	0.71
1:C:3855:ASN:OD1	1:C:3858:ARG:NH2	2.23	0.71
1:D:4130:PRO:O	1:D:4156:ARG:NH1	2.24	0.71
2:I:78:THR:OG1	2:I:80:ASP:OD1	2.07	0.71
1:A:3622:GLY:O	1:A:3626:SER:OG	2.03	0.70
1:D:1683:GLU:OE1	1:D:1683:GLU:N	2.24	0.70
1:B:4130:PRO:O	1:B:4156:ARG:NH1	2.24	0.70
1:A:4130:PRO:O	1:A:4156:ARG:NH1	2.25	0.70
1:C:1683:GLU:N	1:C:1683:GLU:OE1	2.24	0.70
1:C:4130:PRO:O	1:C:4156:ARG:NH1	2.24	0.70
1:A:1683:GLU:OE1	1:A:1683:GLU:N	2.24	0.70
1:B:4633:VAL:O	1:B:4636:THR:OG1	2.08	0.69
1:B:1683:GLU:N	1:B:1683:GLU:OE1	2.24	0.69
1:C:3086:PRO:O	1:C:3090:THR:OG1	2.05	0.69
1:C:4633:VAL:O	1:C:4636:THR:OG1	2.08	0.69
1:B:3086:PRO:O	1:B:3090:THR:OG1	2.05	0.68
1:B:450:GLU:OE1	1:B:450:GLU:N	2.27	0.68
1:D:4633:VAL:O	1:D:4636:THR:OG1	2.07	0.68
2:G:78:THR:OG1	2:G:80:ASP:OD1	2.07	0.68
1:A:87:GLU:OE2	1:A:88:LYS:NZ	2.27	0.68
2:G:74:LYS:NZ	2:G:76:THR:OG1	2.27	0.68
1:A:3086:PRO:O	1:A:3090:THR:OG1	2.05	0.67
1:A:701:GLU:OE2	1:A:1452:GLN:NE2	2.28	0.67
1:B:1434:PRO:O	1:C:2829:ASN:ND2	2.27	0.67
1:D:450:GLU:N	1:D:450:GLU:OE1	2.27	0.67
1:D:87:GLU:OE2	1:D:88:LYS:NZ	2.27	0.67
1:C:450:GLU:N	1:C:450:GLU:OE1	2.27	0.67
1:C:701:GLU:OE2	1:C:1452:GLN:NE2	2.28	0.67
1:A:1100:ARG:NH2	1:A:1234:GLU:O	2.28	0.67
1:A:2829:ASN:ND2	1:D:1434:PRO:O	2.28	0.67
1:B:701:GLU:OE2	1:B:1452:GLN:NE2	2.28	0.67
1:A:450:GLU:N	1:A:450:GLU:OE1	2.27	0.67
1:A:1434:PRO:O	1:B:2829:ASN:ND2	2.28	0.67
1:A:3376:VAL:HG11	1:A:3472:LEU:HD21	1.76	0.67
1:C:87:GLU:OE2	1:C:88:LYS:NZ	2.27	0.67
1:B:87:GLU:OE2	1:B:88:LYS:NZ	2.27	0.67
1:C:3376:VAL:HG11	1:C:3472:LEU:HD21	1.77	0.67
1:D:1100:ARG:NH2	1:D:1234:GLU:O	2.28	0.66
1:C:1434:PRO:O	1:D:2829:ASN:ND2	2.28	0.66
2:I:32:GLN:OE1	2:I:32:GLN:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ARG:NH2	1:B:338:LEU:O	2.29	0.66
1:C:332:ARG:NH2	1:C:338:LEU:O	2.29	0.66
2:J:32:GLN:N	2:J:32:GLN:OE1	2.28	0.66
1:A:332:ARG:NH2	1:A:338:LEU:O	2.29	0.66
1:D:701:GLU:OE2	1:D:1452:GLN:NE2	2.28	0.66
1:B:1100:ARG:NH2	1:B:1234:GLU:O	2.28	0.66
1:B:3376:VAL:HG11	1:B:3472:LEU:HD21	1.76	0.66
1:D:3376:VAL:HG11	1:D:3472:LEU:HD21	1.76	0.66
1:D:69:LEU:HD11	1:D:113:LEU:HD11	1.78	0.66
1:D:332:ARG:NH2	1:D:338:LEU:O	2.29	0.66
1:C:1100:ARG:NH2	1:C:1234:GLU:O	2.28	0.66
1:A:69:LEU:HD11	1:A:113:LEU:HD11	1.78	0.65
2:G:32:GLN:OE1	2:G:32:GLN:N	2.28	0.65
1:C:3285:ASN:OD1	1:C:3286:ASN:ND2	2.30	0.65
1:A:3285:ASN:OD1	1:A:3286:ASN:ND2	2.30	0.65
1:D:3285:ASN:OD1	1:D:3286:ASN:ND2	2.30	0.65
1:D:2240:ASP:OD1	1:D:2296:ARG:NH2	2.30	0.65
2:H:32:GLN:N	2:H:32:GLN:OE1	2.29	0.65
1:D:73:LEU:O	1:D:118:ALA:N	2.30	0.65
1:C:69:LEU:HD11	1:C:113:LEU:HD11	1.78	0.65
1:A:2240:ASP:OD1	1:A:2296:ARG:NH2	2.30	0.65
1:A:1245:ARG:NH1	1:A:1809:ASP:O	2.30	0.64
1:B:3285:ASN:OD1	1:B:3286:ASN:ND2	2.30	0.64
1:D:1245:ARG:NH1	1:D:1809:ASP:O	2.30	0.64
1:D:3086:PRO:O	1:D:3090:THR:OG1	2.05	0.64
1:B:1245:ARG:NH1	1:B:1809:ASP:O	2.30	0.64
1:B:69:LEU:HD11	1:B:113:LEU:HD11	1.78	0.64
1:A:73:LEU:O	1:A:118:ALA:N	2.30	0.64
1:B:2538:GLU:HA	1:B:2583:MET:HE1	1.80	0.64
1:C:73:LEU:O	1:C:118:ALA:N	2.30	0.64
1:A:4562:GLU:OE1	1:A:4562:GLU:N	2.32	0.63
1:A:4633:VAL:O	1:A:4636:THR:OG1	2.08	0.63
1:B:2240:ASP:OD1	1:B:2296:ARG:NH2	2.30	0.63
1:B:73:LEU:O	1:B:118:ALA:N	2.31	0.63
1:C:1245:ARG:NH1	1:C:1809:ASP:O	2.30	0.63
1:D:4562:GLU:OE1	1:D:4562:GLU:N	2.31	0.63
1:C:2240:ASP:OD1	1:C:2296:ARG:NH2	2.30	0.63
1:A:2538:GLU:HA	1:A:2583:MET:HE1	1.80	0.63
1:B:4562:GLU:N	1:B:4562:GLU:OE1	2.31	0.63
1:D:2790:ARG:NH1	1:D:2900:TYR:OH	2.32	0.63
1:C:2538:GLU:HA	1:C:2583:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2790:ARG:NH1	1:C:2900:TYR:OH	2.32	0.63
1:C:4562:GLU:N	1:C:4562:GLU:OE1	2.31	0.63
2:J:74:LYS:NZ	2:J:76:THR:OG1	2.26	0.63
1:B:2790:ARG:NH1	1:B:2900:TYR:OH	2.32	0.62
1:D:903:GLN:O	1:D:915:HIS:N	2.33	0.62
1:D:2762:LEU:O	1:D:2767:LYS:NZ	2.32	0.62
1:D:4026:THR:HG21	1:D:4083:VAL:HG11	1.82	0.62
1:A:2762:LEU:O	1:A:2767:LYS:NZ	2.32	0.62
1:A:2790:ARG:NH1	1:A:2900:TYR:OH	2.32	0.62
1:D:2538:GLU:HA	1:D:2583:MET:HE1	1.80	0.62
1:A:4026:THR:HG21	1:A:4083:VAL:HG11	1.82	0.62
1:C:2762:LEU:O	1:C:2767:LYS:NZ	2.33	0.62
1:A:903:GLN:O	1:A:915:HIS:N	2.33	0.62
1:B:903:GLN:O	1:B:915:HIS:N	2.33	0.62
1:B:1893:LEU:O	1:B:2067:ARG:NH2	2.33	0.61
1:B:4026:THR:HG21	1:B:4083:VAL:HG11	1.82	0.61
1:D:1893:LEU:O	1:D:2067:ARG:NH2	2.33	0.61
1:A:1893:LEU:O	1:A:2067:ARG:NH2	2.33	0.61
1:C:1448:SER:O	1:C:1451:HIS:NE2	2.34	0.61
1:A:1144:ARG:NH1	1:A:1151:HIS:O	2.34	0.61
1:C:3250:GLU:OE1	1:C:3250:GLU:N	2.34	0.61
1:A:3250:GLU:N	1:A:3250:GLU:OE1	2.34	0.61
1:B:1144:ARG:NH1	1:B:1151:HIS:O	2.34	0.61
1:D:1144:ARG:NH1	1:D:1151:HIS:O	2.34	0.61
1:D:1448:SER:O	1:D:1451:HIS:NE2	2.34	0.61
1:D:3250:GLU:N	1:D:3250:GLU:OE1	2.34	0.61
1:A:1448:SER:O	1:A:1451:HIS:NE2	2.34	0.61
1:C:903:GLN:O	1:C:915:HIS:N	2.33	0.60
1:C:1144:ARG:NH1	1:C:1151:HIS:O	2.34	0.60
1:C:4026:THR:HG21	1:C:4083:VAL:HG11	1.82	0.60
1:D:2128:LEU:HA	1:D:2131:VAL:HG12	1.83	0.60
1:B:1448:SER:O	1:B:1451:HIS:NE2	2.34	0.60
1:B:1234:GLU:N	1:B:1234:GLU:OE1	2.35	0.60
1:A:64:ILE:O	1:A:123:HIS:NE2	2.35	0.60
1:A:1234:GLU:N	1:A:1234:GLU:OE1	2.35	0.60
1:C:728:ASP:OD1	1:C:731:HIS:N	2.35	0.60
1:C:1893:LEU:O	1:C:2067:ARG:NH2	2.34	0.60
1:D:728:ASP:OD1	1:D:731:HIS:N	2.35	0.59
1:B:728:ASP:OD1	1:B:731:HIS:N	2.35	0.59
1:A:728:ASP:OD1	1:A:731:HIS:N	2.35	0.59
1:B:2762:LEU:O	1:B:2767:LYS:NZ	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ILE:HD11	1:C:417:ARG:NH1	2.18	0.59
1:D:1931:PHE:O	1:D:1935:LEU:HD22	2.03	0.59
1:A:246:THR:OG1	1:A:247:VAL:N	2.36	0.59
1:B:64:ILE:HD11	1:B:417:ARG:NH1	2.18	0.59
1:C:1234:GLU:OE1	1:C:1234:GLU:N	2.35	0.59
2:H:74:LYS:NZ	2:H:76:THR:OG1	2.26	0.59
1:A:697:TRP:NE1	1:A:757:CYS:SG	2.76	0.59
1:D:64:ILE:O	1:D:123:HIS:NE2	2.35	0.59
1:A:1931:PHE:O	1:A:1935:LEU:HD22	2.03	0.59
1:B:3250:GLU:N	1:B:3250:GLU:OE1	2.34	0.59
1:B:4153:GLU:OE1	1:B:4153:GLU:N	2.36	0.59
1:D:1234:GLU:N	1:D:1234:GLU:OE1	2.35	0.59
1:D:4622:GLU:N	1:D:4622:GLU:OE1	2.36	0.59
1:A:4622:GLU:N	1:A:4622:GLU:OE1	2.36	0.58
1:D:697:TRP:NE1	1:D:757:CYS:SG	2.76	0.58
1:C:4153:GLU:N	1:C:4153:GLU:OE1	2.36	0.58
1:D:1272:ARG:NH2	1:D:1583:CYS:SG	2.77	0.58
1:A:1272:ARG:NH2	1:A:1583:CYS:SG	2.77	0.58
1:B:697:TRP:NE1	1:B:757:CYS:SG	2.76	0.58
1:C:3264:CYS:SG	1:C:3265:THR:N	2.77	0.58
1:A:3264:CYS:SG	1:A:3265:THR:N	2.77	0.58
1:C:697:TRP:NE1	1:C:757:CYS:SG	2.76	0.58
1:C:1931:PHE:O	1:C:1935:LEU:HD22	2.03	0.58
1:C:4185:MET:HE3	1:C:4185:MET:HA	1.85	0.58
1:D:2247:MET:HA	1:D:2247:MET:HE2	1.86	0.58
1:D:4153:GLU:N	1:D:4153:GLU:OE1	2.36	0.58
1:C:1272:ARG:NH2	1:C:1583:CYS:SG	2.76	0.58
1:D:2974:PHE:CE1	1:D:3038:THR:HG21	2.39	0.58
1:D:3264:CYS:SG	1:D:3265:THR:N	2.76	0.58
1:A:4153:GLU:N	1:A:4153:GLU:OE1	2.36	0.58
1:B:1931:PHE:O	1:B:1935:LEU:HD22	2.03	0.58
1:C:246:THR:OG1	1:C:247:VAL:N	2.36	0.58
1:C:64:ILE:O	1:C:123:HIS:NE2	2.36	0.58
1:A:2293:GLU:OE1	1:A:2293:GLU:N	2.37	0.57
1:B:1272:ARG:NH2	1:B:1583:CYS:SG	2.76	0.57
1:B:2974:PHE:CE1	1:B:3038:THR:HG21	2.39	0.57
1:B:3073:ASN:O	1:B:3085:GLN:NE2	2.37	0.57
1:A:2247:MET:HE2	1:A:2247:MET:HA	1.86	0.57
1:B:4185:MET:HA	1:B:4185:MET:HE3	1.85	0.57
1:D:64:ILE:HD11	1:D:417:ARG:NH1	2.18	0.57
1:A:394:HIS:ND1	1:A:396:GLU:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2481:ASP:OD1	1:A:2482:PHE:N	2.38	0.57
1:B:1750:PRO:HD2	1:B:1844:LEU:HD21	1.87	0.57
1:C:3632:GLU:N	1:C:3632:GLU:OE1	2.37	0.57
1:D:3073:ASN:O	1:D:3085:GLN:NE2	2.37	0.57
1:D:4185:MET:HE3	1:D:4185:MET:HA	1.85	0.57
1:A:948:CYS:SG	1:A:949:HIS:N	2.78	0.57
1:C:2481:ASP:OD1	1:C:2482:PHE:N	2.38	0.57
1:D:3632:GLU:OE1	1:D:3632:GLU:N	2.37	0.57
1:A:2974:PHE:CE1	1:A:3038:THR:HG21	2.39	0.57
1:C:3127:VAL:HG22	1:C:3196:LEU:HD11	1.86	0.57
1:B:948:CYS:SG	1:B:949:HIS:N	2.78	0.57
1:B:3632:GLU:OE1	1:B:3632:GLU:N	2.37	0.57
1:B:4622:GLU:OE1	1:B:4622:GLU:N	2.36	0.57
2:G:68:SER:OG	2:G:71:GLN:NE2	2.38	0.57
1:A:3632:GLU:N	1:A:3632:GLU:OE1	2.37	0.57
1:C:222:GLU:N	1:C:222:GLU:OE1	2.38	0.57
1:C:2974:PHE:CE1	1:C:3038:THR:HG21	2.39	0.57
1:D:394:HIS:ND1	1:D:396:GLU:O	2.37	0.57
2:H:68:SER:OG	2:H:71:GLN:NE2	2.37	0.57
1:A:3127:VAL:HG22	1:A:3196:LEU:HD11	1.87	0.57
1:A:64:ILE:HD11	1:A:417:ARG:NH1	2.18	0.57
1:C:1053:ALA:O	1:C:1056:THR:OG1	2.23	0.57
1:C:3469:LEU:O	1:C:3473:LEU:HD23	2.05	0.57
1:D:246:THR:OG1	1:D:247:VAL:N	2.36	0.57
2:J:68:SER:OG	2:J:71:GLN:NE2	2.38	0.57
1:A:563:GLU:N	1:A:563:GLU:OE1	2.38	0.57
1:A:3469:LEU:O	1:A:3473:LEU:HD23	2.05	0.57
1:A:4185:MET:HE3	1:A:4185:MET:HA	1.85	0.57
1:B:2481:ASP:OD1	1:B:2482:PHE:N	2.38	0.57
1:B:3264:CYS:SG	1:B:3265:THR:N	2.77	0.57
1:D:3127:VAL:HG22	1:D:3196:LEU:HD11	1.87	0.57
1:A:1053:ALA:O	1:A:1056:THR:OG1	2.23	0.56
1:B:246:THR:OG1	1:B:247:VAL:N	2.36	0.56
1:B:2293:GLU:N	1:B:2293:GLU:OE1	2.35	0.56
1:D:3469:LEU:O	1:D:3473:LEU:HD23	2.05	0.56
1:A:3073:ASN:O	1:A:3085:GLN:NE2	2.38	0.56
1:B:222:GLU:OE1	1:B:222:GLU:N	2.38	0.56
1:B:2247:MET:HA	1:B:2247:MET:HE2	1.86	0.56
1:B:3900:GLN:O	1:B:3904:ASN:ND2	2.39	0.56
1:C:3073:ASN:O	1:C:3085:GLN:NE2	2.38	0.56
1:D:222:GLU:N	1:D:222:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2481:ASP:OD1	1:D:2482:PHE:N	2.38	0.56
1:B:64:ILE:O	1:B:123:HIS:NE2	2.37	0.56
1:C:2293:GLU:OE1	1:C:2293:GLU:N	2.34	0.56
1:C:4136:GLU:OE2	1:C:4146:ARG:NH1	2.38	0.56
1:D:3985:LEU:HD12	1:D:4100:LEU:HD12	1.88	0.56
1:A:946:LEU:HD22	1:A:998:LYS:HE3	1.88	0.56
1:A:1750:PRO:HD2	1:A:1844:LEU:HD21	1.87	0.56
1:C:394:HIS:ND1	1:C:396:GLU:O	2.38	0.56
1:C:948:CYS:SG	1:C:949:HIS:N	2.78	0.56
1:D:807:ARG:O	1:D:1611:ARG:NH2	2.39	0.56
1:D:946:LEU:HD22	1:D:998:LYS:HE3	1.88	0.56
1:A:807:ARG:O	1:A:1611:ARG:NH2	2.39	0.56
1:B:4136:GLU:OE2	1:B:4146:ARG:NH1	2.38	0.56
1:A:4022:LEU:CD1	1:A:4083:VAL:HG12	2.36	0.56
1:B:770:ILE:O	1:B:770:ILE:HD12	2.06	0.56
1:B:1978:PHE:CZ	1:B:1995:LEU:HD23	2.41	0.56
1:B:4928:ASP:OD2	1:B:4930:THR:OG1	2.24	0.56
1:C:4022:LEU:CD1	1:C:4083:VAL:HG12	2.36	0.56
1:D:1978:PHE:CZ	1:D:1995:LEU:HD23	2.41	0.56
1:B:3127:VAL:HG22	1:B:3196:LEU:HD11	1.87	0.56
1:A:4136:GLU:OE2	1:A:4146:ARG:NH1	2.38	0.56
1:B:323:ASP:O	1:B:327:THR:OG1	2.23	0.56
1:B:3469:LEU:O	1:B:3473:LEU:HD23	2.05	0.56
1:A:441:LYS:NZ	1:A:442:LEU:O	2.29	0.56
1:A:770:ILE:HD12	1:A:770:ILE:O	2.06	0.56
1:A:1978:PHE:CZ	1:A:1995:LEU:HD23	2.41	0.56
1:B:807:ARG:O	1:B:1611:ARG:NH2	2.39	0.56
1:B:2118:LEU:HD22	1:B:2148:ILE:HD13	1.87	0.56
1:C:3985:LEU:HD12	1:C:4100:LEU:HD12	1.88	0.56
1:A:3985:LEU:HD12	1:A:4100:LEU:HD12	1.88	0.55
1:B:3985:LEU:HD12	1:B:4100:LEU:HD12	1.88	0.55
1:B:4022:LEU:CD1	1:B:4083:VAL:HG12	2.36	0.55
1:C:770:ILE:HD12	1:C:770:ILE:O	2.06	0.55
1:C:3851:SER:O	1:C:3855:ASN:ND2	2.39	0.55
1:C:4622:GLU:N	1:C:4622:GLU:OE1	2.36	0.55
1:D:4928:ASP:OD2	1:D:4930:THR:OG1	2.24	0.55
1:C:563:GLU:N	1:C:563:GLU:OE1	2.38	0.55
1:D:4136:GLU:OE2	1:D:4146:ARG:NH1	2.38	0.55
1:C:2247:MET:HE2	1:C:2247:MET:HA	1.86	0.55
1:D:3900:GLN:O	1:D:3904:ASN:ND2	2.39	0.55
1:A:222:GLU:N	1:A:222:GLU:OE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3851:SER:O	1:B:3855:ASN:ND2	2.40	0.55
1:C:4928:ASP:OD2	1:C:4930:THR:OG1	2.24	0.55
1:A:3851:SER:O	1:A:3855:ASN:ND2	2.40	0.55
1:A:3900:GLN:O	1:A:3904:ASN:ND2	2.39	0.55
1:B:494:MET:N	1:B:494:MET:HE2	2.22	0.55
1:C:494:MET:N	1:C:494:MET:HE2	2.22	0.55
1:C:1750:PRO:HD2	1:C:1844:LEU:HD21	1.87	0.55
1:B:394:HIS:ND1	1:B:396:GLU:O	2.38	0.55
1:C:81:MET:O	1:C:85:THR:HG22	2.07	0.55
1:D:565:LEU:HD11	1:D:1585:PRO:CG	2.37	0.55
1:D:1750:PRO:HD2	1:D:1844:LEU:HD21	1.87	0.55
1:D:1979:LYS:NZ	1:D:3630:THR:OG1	2.40	0.55
1:B:565:LEU:HD11	1:B:1585:PRO:CG	2.37	0.55
1:C:1978:PHE:CZ	1:C:1995:LEU:HD23	2.41	0.55
1:D:3851:SER:O	1:D:3855:ASN:ND2	2.40	0.55
1:B:946:LEU:HD22	1:B:998:LYS:HE3	1.88	0.55
1:C:946:LEU:HD22	1:C:998:LYS:HE3	1.88	0.55
1:C:2118:LEU:HD22	1:C:2148:ILE:HD13	1.89	0.55
2:I:68:SER:OG	2:I:71:GLN:NE2	2.38	0.55
1:B:3376:VAL:HG11	1:B:3472:LEU:CD2	2.37	0.54
1:D:770:ILE:HD12	1:D:770:ILE:O	2.06	0.54
1:B:563:GLU:N	1:B:563:GLU:OE1	2.38	0.54
1:C:565:LEU:HD11	1:C:1585:PRO:CG	2.37	0.54
1:D:2118:LEU:HD22	1:D:2148:ILE:HD13	1.88	0.54
1:D:4022:LEU:CD1	1:D:4083:VAL:HG12	2.36	0.54
1:A:3245:MET:HE2	1:A:3272:MET:HE3	1.90	0.54
1:D:2128:LEU:HD23	1:D:2128:LEU:O	2.07	0.54
1:A:565:LEU:HD11	1:A:1585:PRO:CG	2.37	0.54
1:A:2367:SER:OG	1:A:2368:SER:N	2.40	0.54
1:A:3263:CYS:SG	1:A:3264:CYS:N	2.80	0.54
1:A:4928:ASP:OD2	1:A:4930:THR:OG1	2.24	0.54
1:A:81:MET:O	1:A:85:THR:HG22	2.07	0.54
1:C:3376:VAL:HG11	1:C:3472:LEU:CD2	2.38	0.54
1:C:3900:GLN:O	1:C:3904:ASN:ND2	2.40	0.54
1:D:189:GLU:N	1:D:189:GLU:OE1	2.41	0.54
1:D:3245:MET:HE2	1:D:3272:MET:HE3	1.90	0.54
1:C:189:GLU:N	1:C:189:GLU:OE1	2.41	0.54
1:C:807:ARG:O	1:C:1611:ARG:NH2	2.39	0.54
1:C:3245:MET:HE2	1:C:3272:MET:HE3	1.90	0.54
1:D:494:MET:N	1:D:494:MET:HE2	2.21	0.54
1:D:1053:ALA:O	1:D:1056:THR:OG1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2293:GLU:OE1	1:D:2293:GLU:N	2.37	0.54
2:I:74:LYS:NZ	2:I:76:THR:OG1	2.26	0.54
1:A:494:MET:N	1:A:494:MET:HE2	2.22	0.54
1:B:441:LYS:NZ	1:B:442:LEU:O	2.29	0.54
1:B:4589:TYR:OH	1:B:4715:ASP:OD2	2.23	0.54
1:C:3258:GLU:OE2	1:C:3259:ARG:NH1	2.41	0.54
1:B:3258:GLU:OE2	1:B:3259:ARG:NH1	2.41	0.54
1:C:441:LYS:NZ	1:C:442:LEU:O	2.29	0.54
1:B:81:MET:O	1:B:85:THR:HG22	2.08	0.54
1:C:292:GLY:N	1:C:331:PHE:O	2.39	0.54
1:C:323:ASP:O	1:C:327:THR:OG1	2.24	0.54
1:D:81:MET:O	1:D:85:THR:HG22	2.07	0.54
1:D:563:GLU:N	1:D:563:GLU:OE1	2.38	0.54
1:B:4061:GLU:OE1	1:B:4061:GLU:N	2.41	0.53
1:D:3964:ILE:HD12	1:D:3965:GLU:N	2.23	0.53
1:A:3376:VAL:HG11	1:A:3472:LEU:CD2	2.37	0.53
1:B:3799:CYS:O	1:B:3879:ARG:NH2	2.41	0.53
1:D:3009:LYS:O	1:D:3013:LEU:HD22	2.09	0.53
1:A:189:GLU:N	1:A:189:GLU:OE1	2.41	0.53
1:A:1792:THR:HG21	1:A:1825:LEU:HD22	1.89	0.53
1:A:2118:LEU:HD22	1:A:2148:ILE:HD13	1.89	0.53
1:A:3258:GLU:OE2	1:A:3259:ARG:NH1	2.41	0.53
1:A:3799:CYS:O	1:A:3879:ARG:NH2	2.42	0.53
1:D:948:CYS:SG	1:D:949:HIS:N	2.78	0.53
1:C:1574:SER:OG	1:C:1575:GLU:OE1	2.16	0.53
1:D:1792:THR:HG21	1:D:1825:LEU:HD22	1.89	0.53
1:D:3376:VAL:HG11	1:D:3472:LEU:CD2	2.37	0.53
1:B:189:GLU:OE1	1:B:189:GLU:N	2.41	0.53
1:B:3964:ILE:HD12	1:B:3965:GLU:N	2.24	0.53
1:C:1495:SER:O	1:C:1499:GLY:N	2.42	0.53
1:A:2161:MET:SD	1:A:2161:MET:N	2.82	0.53
1:B:1127:GLU:OE1	1:B:1128:LEU:N	2.42	0.53
1:C:2768:GLU:OE2	1:C:2775:LYS:NZ	2.42	0.53
1:C:3009:LYS:O	1:C:3013:LEU:HD22	2.09	0.53
1:D:2161:MET:SD	1:D:2161:MET:N	2.82	0.53
1:A:1127:GLU:OE1	1:A:1128:LEU:N	2.42	0.53
1:B:1792:THR:HG21	1:B:1825:LEU:HD22	1.90	0.53
1:C:717:GLY:N	1:C:720:ASP:OD2	2.42	0.53
1:C:3964:ILE:HD12	1:C:3965:GLU:N	2.24	0.53
1:C:3799:CYS:O	1:C:3879:ARG:NH2	2.42	0.53
1:C:4836:ASP:OD1	1:C:4837:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3258:GLU:OE2	1:D:3259:ARG:NH1	2.41	0.53
1:D:4061:GLU:N	1:D:4061:GLU:OE1	2.41	0.53
1:A:3009:LYS:O	1:A:3013:LEU:HD22	2.09	0.53
1:B:1053:ALA:O	1:B:1056:THR:OG1	2.23	0.53
1:B:4836:ASP:OD1	1:B:4837:GLU:N	2.42	0.53
1:D:1495:SER:O	1:D:1499:GLY:N	2.42	0.53
1:B:1458:ASP:OD1	1:B:1458:ASP:N	2.42	0.52
1:B:2367:SER:OG	1:B:2368:SER:N	2.40	0.52
1:B:3009:LYS:O	1:B:3013:LEU:HD22	2.09	0.52
1:D:292:GLY:N	1:D:331:PHE:O	2.41	0.52
1:A:1458:ASP:N	1:A:1458:ASP:OD1	2.42	0.52
1:A:1495:SER:O	1:A:1499:GLY:N	2.42	0.52
1:A:1979:LYS:NZ	1:A:3630:THR:OG1	2.40	0.52
1:C:2367:SER:OG	1:C:2368:SER:N	2.40	0.52
1:C:1458:ASP:N	1:C:1458:ASP:OD1	2.42	0.52
1:C:1792:THR:HG21	1:C:1825:LEU:HD22	1.89	0.52
1:D:323:ASP:O	1:D:327:THR:OG1	2.24	0.52
2:H:78:THR:OG1	2:H:80:ASP:OD1	2.25	0.52
1:C:1979:LYS:NZ	1:C:3630:THR:OG1	2.40	0.52
1:A:323:ASP:O	1:A:327:THR:OG1	2.24	0.52
1:A:734:SER:O	1:A:1482:ARG:NH1	2.43	0.52
1:A:1463:ARG:O	1:A:1483:SER:OG	2.25	0.52
1:B:1495:SER:O	1:B:1499:GLY:N	2.42	0.52
1:B:1635:GLU:N	1:B:1635:GLU:OE1	2.43	0.52
1:A:3964:ILE:HD12	1:A:3965:GLU:N	2.23	0.52
1:C:1127:GLU:OE1	1:C:1128:LEU:N	2.42	0.52
2:J:78:THR:OG1	2:J:80:ASP:OD1	2.25	0.52
1:A:717:GLY:N	1:A:720:ASP:OD2	2.42	0.52
1:D:814:LEU:HD13	1:D:815:PRO:O	2.09	0.52
1:B:717:GLY:N	1:B:720:ASP:OD2	2.42	0.52
1:C:248:PRO:O	1:C:257:ARG:NE	2.39	0.52
1:A:814:LEU:HD13	1:A:815:PRO:O	2.10	0.52
1:A:4836:ASP:OD1	1:A:4837:GLU:N	2.42	0.52
1:C:814:LEU:HD13	1:C:815:PRO:O	2.09	0.52
1:C:2621:CYS:SG	1:C:2622:LEU:N	2.83	0.52
1:D:441:LYS:NZ	1:D:442:LEU:O	2.29	0.52
1:D:734:SER:O	1:D:1482:ARG:NH1	2.43	0.52
1:D:1649:GLU:N	1:D:1649:GLU:OE1	2.43	0.52
1:B:1979:LYS:NZ	1:B:3630:THR:OG1	2.40	0.52
1:C:1649:GLU:OE1	1:C:1649:GLU:N	2.43	0.52
1:A:1649:GLU:N	1:A:1649:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2470:PHE:CE2	1:D:2474:VAL:HG21	2.45	0.51
1:A:2621:CYS:SG	1:A:2622:LEU:N	2.83	0.51
1:A:2768:GLU:OE2	1:A:2775:LYS:NZ	2.42	0.51
1:B:814:LEU:HD13	1:B:815:PRO:O	2.09	0.51
1:C:734:SER:O	1:C:1482:ARG:NH1	2.43	0.51
1:D:565:LEU:HD11	1:D:1585:PRO:HG3	1.93	0.51
1:D:1127:GLU:OE1	1:D:1128:LEU:N	2.42	0.51
1:A:1446:ILE:O	1:A:1541:PHE:N	2.43	0.51
1:A:565:LEU:HD11	1:A:1585:PRO:HG3	1.93	0.51
1:D:1151:HIS:ND1	1:D:1185:ASP:OD1	2.43	0.51
1:D:1157:GLN:N	1:D:1157:GLN:OE1	2.44	0.51
1:A:399:MET:HE2	1:A:399:MET:H	1.76	0.51
1:B:2621:CYS:SG	1:B:2622:LEU:N	2.83	0.51
1:C:565:LEU:HD11	1:C:1585:PRO:HG3	1.92	0.51
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.43	0.51
1:A:1151:HIS:ND1	1:A:1185:ASP:OD1	2.43	0.51
1:A:4061:GLU:N	1:A:4061:GLU:OE1	2.42	0.51
1:B:778:MET:SD	1:B:779:PHE:N	2.84	0.51
1:B:1649:GLU:N	1:B:1649:GLU:OE1	2.44	0.51
1:C:1157:GLN:OE1	1:C:1157:GLN:N	2.44	0.51
1:D:119:ILE:HD12	1:D:119:ILE:O	2.11	0.51
1:D:4836:ASP:OD1	1:D:4837:GLU:N	2.42	0.51
1:B:2579:LEU:O	1:B:2615:ARG:NH2	2.44	0.51
1:C:399:MET:H	1:C:399:MET:HE2	1.76	0.51
1:C:4061:GLU:N	1:C:4061:GLU:OE1	2.42	0.51
1:A:119:ILE:HD12	1:A:119:ILE:O	2.11	0.51
1:B:292:GLY:N	1:B:331:PHE:O	2.41	0.51
1:B:734:SER:O	1:B:1482:ARG:NH1	2.43	0.51
1:C:455:SER:O	1:C:459:LEU:HD22	2.11	0.51
1:D:455:SER:O	1:D:459:LEU:HD22	2.11	0.51
1:D:3269:SER:OG	1:D:3310:LYS:NZ	2.44	0.51
1:D:3799:CYS:O	1:D:3879:ARG:NH2	2.42	0.51
1:A:1157:GLN:N	1:A:1157:GLN:OE1	2.44	0.51
1:C:1265:HIS:O	1:C:1288:LYS:NZ	2.39	0.51
1:C:1446:ILE:O	1:C:1541:PHE:N	2.43	0.51
1:C:1648:GLN:OE1	1:C:1649:GLU:N	2.44	0.51
1:C:2579:LEU:O	1:C:2615:ARG:NH2	2.43	0.51
1:B:3263:CYS:SG	1:B:3264:CYS:N	2.80	0.50
1:D:399:MET:HE2	1:D:399:MET:H	1.76	0.50
1:D:2621:CYS:SG	1:D:2622:LEU:N	2.83	0.50
1:D:3718:MET:HE2	1:D:3718:MET:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1648:GLN:OE1	1:A:1649:GLU:N	2.44	0.50
1:B:480:ARG:NH1	1:B:3677:GLU:OE1	2.45	0.50
1:D:480:ARG:NH1	1:D:3677:GLU:OE1	2.45	0.50
1:D:1458:ASP:OD1	1:D:1458:ASP:N	2.42	0.50
1:D:1648:GLN:OE1	1:D:1649:GLU:N	2.44	0.50
1:B:565:LEU:HD11	1:B:1585:PRO:HG3	1.93	0.50
1:B:1648:GLN:OE1	1:B:1649:GLU:N	2.44	0.50
1:B:4099:VAL:HG22	1:B:4132:LEU:CD2	2.42	0.50
1:C:778:MET:SD	1:C:779:PHE:N	2.84	0.50
1:D:1446:ILE:O	1:D:1541:PHE:N	2.43	0.50
1:A:480:ARG:NH1	1:A:3677:GLU:OE1	2.45	0.50
1:A:670:TYR:O	1:A:673:TRP:NE1	2.42	0.50
1:A:2470:PHE:CE2	1:A:2474:VAL:HG21	2.45	0.50
1:A:2487:LEU:HD21	1:A:2547:LEU:HG	1.94	0.50
1:B:399:MET:HE2	1:B:399:MET:H	1.76	0.50
1:C:480:ARG:NH1	1:C:3677:GLU:OE1	2.44	0.50
1:C:3718:MET:HA	1:C:3718:MET:HE2	1.93	0.50
1:A:694:ARG:NH1	1:A:718:VAL:O	2.44	0.50
1:A:4020:LEU:HD22	1:A:4127:TYR:CE2	2.47	0.50
1:B:1157:GLN:N	1:B:1157:GLN:OE1	2.44	0.50
1:B:2470:PHE:CE2	1:B:2474:VAL:HG21	2.46	0.50
1:B:2768:GLU:OE2	1:B:2775:LYS:NZ	2.42	0.50
1:C:119:ILE:HD12	1:C:119:ILE:O	2.11	0.50
1:C:270:HIS:O	1:C:273:SER:OG	2.29	0.50
1:B:119:ILE:HD12	1:B:119:ILE:O	2.11	0.50
1:C:694:ARG:NH1	1:C:718:VAL:O	2.44	0.50
1:C:1635:GLU:OE1	1:C:1635:GLU:N	2.43	0.50
1:C:2470:PHE:CE2	1:C:2474:VAL:HG21	2.45	0.50
1:C:3939:LEU:HD21	1:C:3980:MET:HE1	1.92	0.50
1:D:2768:GLU:OE2	1:D:2775:LYS:NZ	2.43	0.50
1:D:4020:LEU:HD22	1:D:4127:TYR:CE2	2.47	0.50
1:B:670:TYR:O	1:B:673:TRP:NE1	2.42	0.50
1:B:2487:LEU:HD21	1:B:2547:LEU:HG	1.94	0.50
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.43	0.50
1:A:3272:MET:SD	1:A:3272:MET:N	2.85	0.50
1:B:455:SER:O	1:B:459:LEU:HD22	2.11	0.50
1:C:2487:LEU:HD21	1:C:2547:LEU:HG	1.94	0.50
1:C:3272:MET:SD	1:C:3272:MET:N	2.85	0.50
1:D:778:MET:SD	1:D:779:PHE:N	2.84	0.50
1:D:2487:LEU:HD21	1:D:2547:LEU:HG	1.94	0.50
1:A:778:MET:SD	1:A:779:PHE:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ARG:NH1	1:B:718:VAL:O	2.44	0.50
1:D:694:ARG:NH1	1:D:718:VAL:O	2.44	0.50
1:D:717:GLY:N	1:D:720:ASP:OD2	2.42	0.50
1:D:2579:LEU:O	1:D:2615:ARG:NH2	2.44	0.50
1:B:983:LEU:O	1:B:1055:ARG:NH1	2.44	0.49
1:C:3042:ARG:NH2	1:C:3115:GLN:O	2.45	0.49
1:C:4099:VAL:HG22	1:C:4132:LEU:CD2	2.42	0.49
1:D:1635:GLU:OE1	1:D:1635:GLU:N	2.43	0.49
1:C:2128:LEU:HA	1:C:2131:VAL:HG12	1.94	0.49
1:C:2791:THR:HG22	1:C:2899:GLY:O	2.13	0.49
1:C:3263:CYS:SG	1:C:3264:CYS:N	2.80	0.49
1:D:3042:ARG:NH2	1:D:3115:GLN:O	2.45	0.49
1:D:4099:VAL:HG22	1:D:4132:LEU:CD2	2.42	0.49
2:H:38:ASP:OD1	2:H:39:SER:N	2.45	0.49
1:A:3718:MET:HA	1:A:3718:MET:HE2	1.94	0.49
1:B:1909:LEU:HB2	1:B:2086:LEU:HD11	1.95	0.49
1:B:2128:LEU:HA	1:B:2131:VAL:HG12	1.94	0.49
1:D:2791:THR:HG22	1:D:2899:GLY:O	2.13	0.49
2:G:80:ASP:OD1	2:G:81:VAL:N	2.45	0.49
1:A:455:SER:O	1:A:459:LEU:HD22	2.11	0.49
1:A:2418:ILE:HD12	1:A:2419:ARG:N	2.27	0.49
1:A:2579:LEU:O	1:A:2615:ARG:NH2	2.44	0.49
1:B:270:HIS:O	1:B:273:SER:OG	2.29	0.49
1:B:3718:MET:HE2	1:B:3718:MET:HA	1.94	0.49
2:H:39:SER:OG	2:H:42:ASP:N	2.45	0.49
1:A:1786:ASP:OD1	1:A:1787:ILE:N	2.46	0.49
1:B:2418:ILE:HD12	1:B:2419:ARG:N	2.27	0.49
1:B:3245:MET:HE2	1:B:3272:MET:HE3	1.94	0.49
1:B:3939:LEU:HD21	1:B:3980:MET:HE1	1.95	0.49
1:C:314:LEU:HD11	1:C:372:LEU:HD23	1.93	0.49
1:C:2418:ILE:HD12	1:C:2419:ARG:N	2.27	0.49
1:D:270:HIS:O	1:D:273:SER:OG	2.29	0.49
1:D:3272:MET:SD	1:D:3272:MET:N	2.85	0.49
2:I:39:SER:OG	2:I:42:ASP:N	2.45	0.49
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.43	0.49
1:A:3042:ARG:NH2	1:A:3115:GLN:O	2.45	0.49
1:A:3629:GLU:OE1	1:A:3629:GLU:N	2.46	0.49
1:B:3234:MET:SD	1:B:3234:MET:N	2.86	0.49
1:B:3272:MET:SD	1:B:3272:MET:N	2.86	0.49
1:C:4092:ASP:OD1	1:C:4093:ILE:N	2.46	0.49
1:D:670:TYR:O	1:D:673:TRP:NE1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:80:ASP:OD1	2:I:81:VAL:N	2.46	0.49
1:A:270:HIS:O	1:A:273:SER:OG	2.30	0.49
1:A:292:GLY:N	1:A:331:PHE:O	2.41	0.49
1:B:4020:LEU:HD22	1:B:4127:TYR:CE2	2.47	0.49
1:B:4092:ASP:OD1	1:B:4093:ILE:N	2.46	0.49
1:C:1909:LEU:HB2	1:C:2086:LEU:HD11	1.95	0.49
1:C:1932:VAL:HG21	1:C:3616:VAL:HA	1.95	0.49
1:C:2383:MET:SD	1:C:2383:MET:N	2.86	0.49
1:D:586:LEU:HD22	1:D:625:VAL:HG21	1.95	0.49
1:D:2418:ILE:HD12	1:D:2419:ARG:N	2.27	0.49
2:G:39:SER:OG	2:G:42:ASP:N	2.45	0.49
1:A:1909:LEU:HB2	1:A:2086:LEU:HD11	1.95	0.49
1:B:1265:HIS:O	1:B:1288:LYS:NZ	2.39	0.49
1:C:670:TYR:O	1:C:673:TRP:NE1	2.42	0.49
1:C:1151:HIS:ND1	1:C:1185:ASP:OD1	2.43	0.49
1:D:1786:ASP:OD1	1:D:1787:ILE:N	2.46	0.49
1:A:1635:GLU:OE1	1:A:1635:GLU:N	2.43	0.49
1:D:2592:VAL:HG22	1:D:2643:LEU:HG	1.95	0.49
1:A:2791:THR:HG22	1:A:2899:GLY:O	2.13	0.48
1:B:248:PRO:O	1:B:257:ARG:NE	2.39	0.48
1:B:1151:HIS:ND1	1:B:1185:ASP:OD1	2.44	0.48
1:B:2383:MET:SD	1:B:2383:MET:N	2.86	0.48
1:C:797:GLY:N	1:C:1622:CYS:O	2.46	0.48
1:C:983:LEU:O	1:C:1055:ARG:NH1	2.44	0.48
1:C:3234:MET:SD	1:C:3234:MET:N	2.86	0.48
1:C:4020:LEU:HD22	1:C:4127:TYR:CE2	2.47	0.48
1:A:2128:LEU:HA	1:A:2131:VAL:HG12	1.94	0.48
1:B:2791:THR:HG22	1:B:2899:GLY:O	2.13	0.48
1:C:309:MET:SD	1:C:309:MET:N	2.87	0.48
1:C:2592:VAL:HG22	1:C:2643:LEU:HG	1.96	0.48
1:B:2065:MET:HA	1:B:2065:MET:HE2	1.96	0.48
1:D:2128:LEU:HD21	1:D:2137:GLU:HB3	1.95	0.48
1:A:3233:MET:O	1:A:3237:VAL:N	2.47	0.48
1:A:4099:VAL:HG22	1:A:4132:LEU:CD2	2.42	0.48
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.43	0.48
1:B:3042:ARG:NH2	1:B:3115:GLN:O	2.45	0.48
1:B:3233:MET:O	1:B:3237:VAL:N	2.46	0.48
1:C:779:PHE:HE1	1:C:1467:VAL:HG22	1.78	0.48
1:D:3629:GLU:N	1:D:3629:GLU:OE1	2.46	0.48
1:A:586:LEU:HD22	1:A:625:VAL:HG21	1.96	0.48
1:C:3233:MET:O	1:C:3237:VAL:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:ASP:OD1	2:G:39:SER:N	2.46	0.48
1:A:309:MET:SD	1:A:309:MET:N	2.87	0.48
1:A:1950:LEU:HD13	1:A:1957:THR:HA	1.96	0.48
1:B:87:GLU:OE1	1:B:87:GLU:N	2.42	0.48
1:B:3899:GLU:OE1	1:B:3903:ARG:NH2	2.46	0.48
1:C:1124:PRO:HD2	1:C:1595:VAL:HG23	1.96	0.48
1:C:2065:MET:HE2	1:C:2065:MET:HA	1.96	0.48
1:D:309:MET:SD	1:D:309:MET:N	2.87	0.48
1:D:779:PHE:HE1	1:D:1467:VAL:HG22	1.79	0.48
1:D:1909:LEU:HB2	1:D:2086:LEU:HD11	1.95	0.48
1:D:1950:LEU:HD13	1:D:1957:THR:HA	1.96	0.48
1:D:2383:MET:SD	1:D:2383:MET:N	2.86	0.48
1:A:3234:MET:SD	1:A:3234:MET:N	2.86	0.48
1:B:779:PHE:HE1	1:B:1467:VAL:HG22	1.79	0.48
1:B:797:GLY:N	1:B:1622:CYS:O	2.46	0.48
1:C:1893:LEU:CD1	1:C:2060:LEU:HD11	2.44	0.48
1:D:234:LEU:HD11	1:D:356:TYR:HE1	1.79	0.48
1:D:797:GLY:N	1:D:1622:CYS:O	2.46	0.48
1:D:3899:GLU:OE1	1:D:3903:ARG:NH2	2.47	0.48
1:A:234:LEU:HD11	1:A:356:TYR:HE1	1.79	0.48
1:A:983:LEU:O	1:A:1055:ARG:NH1	2.44	0.48
1:D:1575:GLU:OE1	1:D:1575:GLU:N	2.47	0.48
1:D:1932:VAL:HG21	1:D:3616:VAL:HA	1.95	0.48
1:D:2337:GLU:OE1	1:D:2337:GLU:N	2.46	0.48
1:D:2423:ARG:O	1:D:2475:TYR:OH	2.30	0.48
2:I:38:ASP:OD1	2:I:39:SER:N	2.46	0.48
1:A:797:GLY:N	1:A:1622:CYS:O	2.46	0.48
1:A:4609:LEU:HD21	1:A:4669:LEU:HD21	1.95	0.48
1:B:1215:MET:HE3	1:B:1215:MET:HA	1.96	0.48
1:B:1950:LEU:HD13	1:B:1957:THR:HA	1.96	0.48
1:D:3939:LEU:HD21	1:D:3980:MET:HE1	1.95	0.48
1:D:4078:ASP:OD1	1:D:4078:ASP:N	2.46	0.48
1:D:4609:LEU:HD21	1:D:4669:LEU:HD21	1.95	0.48
1:A:779:PHE:HE1	1:A:1467:VAL:HG22	1.78	0.48
1:A:1932:VAL:HG21	1:A:3616:VAL:HA	1.95	0.48
1:A:2383:MET:SD	1:A:2383:MET:N	2.86	0.48
1:A:2592:VAL:HG22	1:A:2643:LEU:HG	1.96	0.48
1:A:3899:GLU:OE1	1:A:3903:ARG:NH2	2.47	0.48
1:B:309:MET:N	1:B:309:MET:SD	2.87	0.48
1:B:744:PRO:O	1:B:745:ASN:ND2	2.40	0.48
1:C:234:LEU:HD11	1:C:356:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3039:LEU:O	1:C:3110:HIS:NE2	2.47	0.48
1:C:3899:GLU:OE1	1:C:3903:ARG:NH2	2.47	0.48
1:C:4078:ASP:OD1	1:C:4078:ASP:N	2.46	0.48
1:D:4607:ARG:NH2	1:D:4643:TYR:OH	2.47	0.48
1:B:1786:ASP:OD1	1:B:1787:ILE:N	2.45	0.47
1:B:2680:MET:HE3	1:B:2680:MET:HA	1.96	0.47
1:C:3629:GLU:OE1	1:C:3629:GLU:N	2.46	0.47
1:D:3039:LEU:O	1:D:3110:HIS:NE2	2.47	0.47
2:J:38:ASP:OD1	2:J:39:SER:N	2.46	0.47
1:A:2435:ILE:O	1:A:2464:LYS:NZ	2.40	0.47
1:A:3039:LEU:O	1:A:3110:HIS:NE2	2.47	0.47
1:A:4092:ASP:OD1	1:A:4093:ILE:N	2.47	0.47
1:D:314:LEU:HD11	1:D:372:LEU:HD23	1.95	0.47
1:D:993:GLU:OE1	1:D:1051:ARG:NH1	2.47	0.47
1:A:1124:PRO:HD2	1:A:1595:VAL:HG23	1.96	0.47
1:A:4050:ALA:O	1:A:4053:SER:OG	2.28	0.47
1:B:586:LEU:HD22	1:B:625:VAL:HG21	1.96	0.47
1:C:1950:LEU:HD13	1:C:1957:THR:HA	1.95	0.47
1:C:2680:MET:HE3	1:C:2680:MET:HA	1.97	0.47
1:D:3233:MET:O	1:D:3237:VAL:N	2.47	0.47
1:B:2592:VAL:HG22	1:B:2643:LEU:HG	1.95	0.47
1:B:3039:LEU:O	1:B:3110:HIS:NE2	2.47	0.47
1:D:983:LEU:O	1:D:1055:ARG:NH1	2.44	0.47
1:D:1463:ARG:O	1:D:1483:SER:OG	2.26	0.47
1:D:1893:LEU:CD1	1:D:2060:LEU:HD11	2.44	0.47
1:A:1265:HIS:O	1:A:1288:LYS:NZ	2.39	0.47
1:D:1124:PRO:HD2	1:D:1595:VAL:HG23	1.96	0.47
1:D:3234:MET:SD	1:D:3234:MET:N	2.86	0.47
1:A:314:LEU:HD11	1:A:372:LEU:HD23	1.96	0.47
1:A:2065:MET:HE2	1:A:2065:MET:HA	1.96	0.47
1:A:3939:LEU:HD21	1:A:3980:MET:HE1	1.95	0.47
1:B:1932:VAL:HG21	1:B:3616:VAL:HA	1.95	0.47
1:B:2423:ARG:O	1:B:2475:TYR:OH	2.31	0.47
1:B:2635:GLU:O	1:B:2639:LEU:HD22	2.15	0.47
1:C:586:LEU:HD22	1:C:625:VAL:HG21	1.96	0.47
1:C:4609:LEU:HD21	1:C:4669:LEU:HD21	1.95	0.47
1:D:248:PRO:O	1:D:257:ARG:NE	2.39	0.47
1:D:4092:ASP:OD1	1:D:4093:ILE:N	2.47	0.47
1:A:207:PHE:CZ	1:B:2324:ILE:HD13	2.49	0.47
1:A:1168:MET:SD	1:A:1168:MET:N	2.86	0.47
1:A:1893:LEU:CD1	1:A:2060:LEU:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2635:GLU:O	1:A:2639:LEU:HD22	2.15	0.47
1:B:234:LEU:HD11	1:B:356:TYR:HE1	1.79	0.47
1:B:1124:PRO:HD2	1:B:1595:VAL:HG23	1.96	0.47
1:B:1893:LEU:CD1	1:B:2060:LEU:HD11	2.44	0.47
1:B:2268:LEU:HD21	1:B:2298:LEU:CD2	2.45	0.47
1:B:3629:GLU:N	1:B:3629:GLU:OE1	2.46	0.47
1:B:4609:LEU:HD21	1:B:4669:LEU:HD21	1.95	0.47
1:C:1099:GLY:O	1:C:1169:ASN:ND2	2.48	0.47
1:C:2485:HIS:O	1:C:2489:VAL:HG12	2.15	0.47
1:D:3376:VAL:HG12	1:D:3383:TRP:HZ3	1.80	0.47
1:B:2485:HIS:O	1:B:2489:VAL:HG12	2.15	0.47
1:C:1446:ILE:HG21	1:C:1545:PHE:HZ	1.80	0.47
1:C:2268:LEU:HD21	1:C:2298:LEU:CD2	2.45	0.47
1:C:2635:GLU:O	1:C:2639:LEU:HD22	2.15	0.47
1:D:2635:GLU:O	1:D:2639:LEU:HD22	2.15	0.47
2:J:39:SER:OG	2:J:42:ASP:N	2.45	0.47
1:A:248:PRO:O	1:A:257:ARG:NE	2.39	0.47
1:A:1099:GLY:O	1:A:1169:ASN:ND2	2.48	0.47
1:A:2268:LEU:HD21	1:A:2298:LEU:CD2	2.45	0.47
1:B:1099:GLY:O	1:B:1169:ASN:ND2	2.48	0.47
1:C:168:GLN:N	1:C:168:GLN:OE1	2.48	0.47
1:C:1575:GLU:OE1	1:C:1575:GLU:N	2.46	0.47
1:C:1786:ASP:OD1	1:C:1787:ILE:N	2.45	0.47
1:B:207:PHE:CZ	1:C:2324:ILE:HD13	2.50	0.47
1:C:993:GLU:OE1	1:C:1051:ARG:NH1	2.48	0.47
1:D:2065:MET:HA	1:D:2065:MET:HE2	1.96	0.47
1:D:2268:LEU:HD21	1:D:2298:LEU:CD2	2.45	0.47
1:A:1575:GLU:OE1	1:A:1575:GLU:N	2.47	0.46
1:A:2485:HIS:O	1:A:2489:VAL:HG12	2.15	0.46
1:A:3376:VAL:HG12	1:A:3383:TRP:HZ3	1.80	0.46
1:C:66:THR:HG23	1:C:124:SER:OG	2.15	0.46
1:C:676:GLU:OE1	1:C:812:LYS:N	2.48	0.46
1:C:4607:ARG:NH2	1:C:4643:TYR:OH	2.46	0.46
1:D:661:LEU:O	1:D:788:PHE:N	2.46	0.46
1:D:2680:MET:HE3	1:D:2680:MET:HA	1.96	0.46
1:D:2714:GLU:OE1	1:D:2714:GLU:N	2.48	0.46
1:A:993:GLU:OE1	1:A:1051:ARG:NH1	2.48	0.46
1:C:364:GLN:NE2	1:C:369:GLY:O	2.45	0.46
1:C:2588:LEU:O	1:C:2592:VAL:HG23	2.15	0.46
1:D:1099:GLY:O	1:D:1169:ASN:ND2	2.48	0.46
1:D:4087:HIS:O	1:D:4091:LYS:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3682:GLU:OE1	1:A:3682:GLU:N	2.48	0.46
1:A:4663:ASP:OD1	1:A:4664:ARG:N	2.49	0.46
1:A:1272:ARG:NH1	1:A:1587:LEU:O	2.49	0.46
1:A:2680:MET:HE3	1:A:2680:MET:HA	1.96	0.46
1:B:2714:GLU:OE1	1:B:2714:GLU:N	2.48	0.46
1:C:2423:ARG:O	1:C:2475:TYR:OH	2.31	0.46
1:D:2367:SER:OG	1:D:2368:SER:N	2.40	0.46
1:A:676:GLU:OE1	1:A:812:LYS:N	2.47	0.46
1:A:1446:ILE:HG21	1:A:1545:PHE:HZ	1.80	0.46
1:B:314:LEU:HD11	1:B:372:LEU:HD23	1.96	0.46
1:B:1958:ALA:O	1:B:1965:ARG:NH2	2.49	0.46
1:C:3376:VAL:HG12	1:C:3383:TRP:HZ3	1.80	0.46
1:D:168:GLN:N	1:D:168:GLN:OE1	2.48	0.46
1:D:2470:PHE:CZ	1:D:2474:VAL:HG21	2.51	0.46
1:D:4663:ASP:OD1	1:D:4664:ARG:N	2.49	0.46
1:A:168:GLN:N	1:A:168:GLN:OE1	2.49	0.46
1:B:993:GLU:OE1	1:B:1051:ARG:NH1	2.48	0.46
1:B:1103:PHE:CE2	1:B:1215:MET:HE1	2.50	0.46
1:C:207:PHE:CZ	1:D:2324:ILE:HD13	2.51	0.46
1:C:2161:MET:SD	1:C:2161:MET:N	2.88	0.46
1:C:4663:ASP:OD1	1:C:4664:ARG:N	2.49	0.46
1:A:2470:PHE:CZ	1:A:2474:VAL:HG21	2.50	0.46
1:A:2588:LEU:O	1:A:2592:VAL:HG23	2.15	0.46
1:C:2848:HIS:CE1	1:C:2876:LEU:HD11	2.51	0.46
1:A:2848:HIS:CE1	1:A:2876:LEU:HD11	2.51	0.46
1:A:3269:SER:OG	1:A:3310:LYS:NZ	2.44	0.46
1:A:4583:PHE:N	1:A:4725:MET:HE1	2.31	0.46
1:B:2251:GLU:OE1	1:B:2251:GLU:N	2.46	0.46
1:B:3682:GLU:OE1	1:B:3682:GLU:N	2.49	0.46
1:C:19:GLU:N	1:C:218:SER:O	2.48	0.46
1:D:1446:ILE:HG21	1:D:1545:PHE:HZ	1.80	0.46
1:B:1708:ILE:HD13	1:B:1712:LEU:HD12	1.98	0.46
1:B:1708:ILE:HG23	1:B:1828:THR:HG21	1.98	0.46
1:B:3943:VAL:HG11	1:B:4001:MET:HE2	1.97	0.46
1:C:2337:GLU:OE1	1:C:2337:GLU:N	2.46	0.46
1:C:2470:PHE:CZ	1:C:2474:VAL:HG21	2.50	0.46
1:D:1272:ARG:NH1	1:D:1587:LEU:O	2.49	0.46
1:D:2435:ILE:O	1:D:2464:LYS:NZ	2.40	0.46
1:A:4087:HIS:O	1:A:4091:LYS:N	2.43	0.46
1:B:1931:PHE:CZ	1:B:1995:LEU:HD22	2.51	0.46
1:B:4663:ASP:OD1	1:B:4664:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1708:ILE:HD13	1:C:1712:LEU:HD12	1.98	0.46
1:C:2251:GLU:OE1	1:C:2251:GLU:N	2.46	0.46
1:C:3612:ARG:O	1:C:3616:VAL:HG23	2.16	0.46
1:D:78:LEU:HD21	1:D:186:VAL:HG21	1.98	0.46
1:A:1958:ALA:O	1:A:1965:ARG:NH2	2.49	0.45
1:A:2324:ILE:HD13	1:D:207:PHE:CZ	2.51	0.45
1:A:3762:ILE:HD11	1:A:3837:ASP:O	2.16	0.45
1:A:4607:ARG:NH2	1:A:4643:TYR:OH	2.47	0.45
1:B:168:GLN:OE1	1:B:168:GLN:N	2.49	0.45
1:B:1021:GLN:OE1	1:B:1022:GLN:N	2.50	0.45
1:B:2848:HIS:CE1	1:B:2876:LEU:HD11	2.51	0.45
1:C:1931:PHE:CZ	1:C:1995:LEU:HD22	2.51	0.45
1:C:2298:LEU:HD13	1:C:2394:LEU:HA	1.98	0.45
1:D:890:HIS:NE2	1:D:919:VAL:O	2.49	0.45
1:D:2485:HIS:O	1:D:2489:VAL:HG12	2.15	0.45
1:A:890:HIS:NE2	1:A:919:VAL:O	2.49	0.45
1:B:1272:ARG:NH1	1:B:1587:LEU:O	2.49	0.45
1:D:1021:GLN:OE1	1:D:1022:GLN:N	2.49	0.45
1:D:1267:HIS:O	1:D:1288:LYS:N	2.47	0.45
1:D:1931:PHE:CZ	1:D:1995:LEU:HD22	2.51	0.45
1:D:2298:LEU:HD13	1:D:2394:LEU:HA	1.98	0.45
1:D:4583:PHE:N	1:D:4725:MET:HE1	2.31	0.45
1:A:744:PRO:O	1:A:745:ASN:ND2	2.41	0.45
1:A:1105:PHE:CB	1:A:1115:VAL:HG21	2.47	0.45
1:A:1708:ILE:HD13	1:A:1712:LEU:HD12	1.98	0.45
1:A:1708:ILE:HG23	1:A:1828:THR:HG21	1.98	0.45
1:A:2569:GLU:OE1	1:A:2570:VAL:HG13	2.16	0.45
1:B:676:GLU:OE1	1:B:812:LYS:N	2.48	0.45
1:B:1722:MET:SD	1:B:1722:MET:N	2.89	0.45
1:B:2588:LEU:O	1:B:2592:VAL:HG23	2.15	0.45
1:C:1958:ALA:O	1:C:1965:ARG:NH2	2.49	0.45
1:C:2414:GLU:OE1	1:C:2414:GLU:N	2.47	0.45
1:C:3854:GLN:NE2	1:C:3921:GLU:O	2.49	0.45
1:D:1708:ILE:HG23	1:D:1828:THR:HG21	1.98	0.45
1:D:1958:ALA:O	1:D:1965:ARG:NH2	2.49	0.45
1:D:2187:THR:HG23	1:D:2188:PHE:CD2	2.52	0.45
2:J:80:ASP:OD1	2:J:81:VAL:N	2.50	0.45
1:A:87:GLU:OE1	1:A:87:GLU:N	2.42	0.45
1:A:2414:GLU:OE1	1:A:2414:GLU:N	2.47	0.45
1:A:3854:GLN:NE2	1:A:3921:GLU:O	2.50	0.45
1:B:641:ASP:OD1	1:B:641:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2569:GLU:OE1	1:B:2570:VAL:HG13	2.16	0.45
1:C:4583:PHE:N	1:C:4725:MET:HE1	2.31	0.45
1:D:1708:ILE:HD13	1:D:1712:LEU:HD12	1.98	0.45
1:D:2588:LEU:O	1:D:2592:VAL:HG23	2.15	0.45
1:D:3762:ILE:HD11	1:D:3837:ASP:O	2.16	0.45
1:A:3943:VAL:HG11	1:A:4001:MET:HE2	1.98	0.45
1:B:2470:PHE:CZ	1:B:2474:VAL:HG21	2.51	0.45
1:B:3376:VAL:HG12	1:B:3383:TRP:HZ3	1.80	0.45
1:B:3900:GLN:OE1	1:B:3903:ARG:NH2	2.49	0.45
1:C:1105:PHE:CB	1:C:1115:VAL:HG21	2.47	0.45
1:C:3900:GLN:OE1	1:C:3903:ARG:NH2	2.50	0.45
1:D:1105:PHE:CB	1:D:1115:VAL:HG21	2.47	0.45
1:D:4136:GLU:O	1:D:4917:TYR:OH	2.34	0.45
1:A:3612:ARG:O	1:A:3616:VAL:HG23	2.17	0.45
1:A:4078:ASP:OD1	1:A:4078:ASP:N	2.46	0.45
1:B:754:VAL:C	1:B:755:ILE:HD12	2.42	0.45
1:B:1446:ILE:HG21	1:B:1545:PHE:HZ	1.80	0.45
1:B:1446:ILE:O	1:B:1541:PHE:N	2.43	0.45
1:B:4583:PHE:N	1:B:4725:MET:HE1	2.31	0.45
1:B:4607:ARG:NH2	1:B:4643:TYR:OH	2.47	0.45
1:C:78:LEU:HD21	1:C:186:VAL:HG21	1.98	0.45
1:C:1722:MET:N	1:C:1722:MET:SD	2.90	0.45
1:A:19:GLU:N	1:A:218:SER:O	2.48	0.45
1:A:1650:GLU:OE1	1:A:1651:LEU:HD22	2.17	0.45
1:A:1722:MET:SD	1:A:1722:MET:N	2.90	0.45
1:A:2187:THR:HG23	1:A:2188:PHE:CD2	2.52	0.45
1:C:754:VAL:C	1:C:755:ILE:HD12	2.42	0.45
1:D:3612:ARG:O	1:D:3616:VAL:HG23	2.16	0.45
1:D:3943:VAL:HG11	1:D:4001:MET:HE2	1.98	0.45
2:H:80:ASP:OD1	2:H:81:VAL:N	2.49	0.45
1:A:641:ASP:OD1	1:A:641:ASP:N	2.50	0.45
1:A:1947:MET:HE3	1:A:1947:MET:HA	1.99	0.45
1:B:1947:MET:HA	1:B:1947:MET:HE3	1.99	0.45
1:B:3269:SER:OG	1:B:3310:LYS:NZ	2.44	0.45
1:B:4078:ASP:OD1	1:B:4078:ASP:N	2.46	0.45
1:C:625:VAL:HG22	1:C:2132:ARG:HD3	1.99	0.45
1:C:1595:VAL:HG13	1:C:1595:VAL:O	2.17	0.45
1:C:2187:THR:HG23	1:C:2188:PHE:CD2	2.52	0.45
1:D:1650:GLU:OE1	1:D:1651:LEU:HD22	2.17	0.45
1:A:234:LEU:HD11	1:A:356:TYR:CE1	2.52	0.45
1:B:3612:ARG:O	1:B:3616:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3943:VAL:HG11	1:C:4001:MET:HE2	1.98	0.45
1:D:754:VAL:C	1:D:755:ILE:HD12	2.42	0.45
1:A:2298:LEU:HD13	1:A:2394:LEU:HA	1.98	0.45
1:B:1575:GLU:OE1	1:B:1575:GLU:N	2.47	0.45
1:C:1272:ARG:NH1	1:C:1587:LEU:O	2.49	0.45
1:C:1650:GLU:OE1	1:C:1651:LEU:HD22	2.17	0.45
1:D:879:GLU:OE2	1:D:882:ARG:NH2	2.50	0.45
1:D:1595:VAL:O	1:D:1595:VAL:HG13	2.17	0.45
1:D:2569:GLU:OE1	1:D:2570:VAL:HG13	2.16	0.45
1:D:4050:ALA:O	1:D:4053:SER:OG	2.28	0.45
1:A:754:VAL:C	1:A:755:ILE:HD12	2.42	0.44
1:A:1931:PHE:CZ	1:A:1995:LEU:HD22	2.51	0.44
1:B:78:LEU:HD21	1:B:186:VAL:HG21	1.99	0.44
1:C:4058:THR:O	1:C:4062:THR:OG1	2.31	0.44
1:D:87:GLU:OE1	1:D:87:GLU:N	2.42	0.44
1:D:1722:MET:SD	1:D:1722:MET:N	2.90	0.44
1:D:2848:HIS:CE1	1:D:2876:LEU:HD11	2.51	0.44
1:A:1595:VAL:HG13	1:A:1595:VAL:O	2.17	0.44
1:B:1105:PHE:CB	1:B:1115:VAL:HG21	2.47	0.44
1:D:3346:ASP:OD1	1:D:3347:MET:N	2.51	0.44
1:A:1988:PRO:CG	1:A:1991:ILE:HD12	2.47	0.44
1:C:375:GLN:HG2	1:C:377:VAL:HG13	2.00	0.44
1:C:1021:GLN:OE1	1:C:1022:GLN:N	2.50	0.44
1:C:1947:MET:HE3	1:C:1947:MET:HA	1.99	0.44
1:C:1988:PRO:CG	1:C:1991:ILE:HD12	2.47	0.44
1:D:234:LEU:HD11	1:D:356:TYR:CE1	2.52	0.44
1:D:625:VAL:HG22	1:D:2132:ARG:HD3	2.00	0.44
1:A:3346:ASP:OD1	1:A:3347:MET:N	2.51	0.44
1:B:2414:GLU:OE1	1:B:2414:GLU:N	2.47	0.44
1:C:641:ASP:OD1	1:C:641:ASP:N	2.50	0.44
1:D:1555:GLN:NE2	1:D:1557:GLU:OE2	2.48	0.44
1:D:3682:GLU:N	1:D:3682:GLU:OE1	2.48	0.44
1:B:625:VAL:HG22	1:B:2132:ARG:HD3	1.98	0.44
1:B:1168:MET:SD	1:B:1168:MET:N	2.86	0.44
1:B:3762:ILE:HD11	1:B:3837:ASP:O	2.17	0.44
1:B:4058:THR:O	1:B:4062:THR:OG1	2.31	0.44
1:C:744:PRO:O	1:C:745:ASN:ND2	2.41	0.44
1:C:3762:ILE:HD11	1:C:3837:ASP:O	2.17	0.44
1:A:655:MET:CE	1:A:834:VAL:HG12	2.48	0.44
1:A:879:GLU:OE2	1:A:882:ARG:NH2	2.51	0.44
1:B:1595:VAL:HG13	1:B:1595:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1708:ILE:HD11	1:B:1825:LEU:HA	2.00	0.44
1:B:1756:THR:N	1:B:1922:GLU:OE2	2.51	0.44
1:B:2394:LEU:O	1:B:2398:LEU:HD22	2.18	0.44
1:B:3346:ASP:OD1	1:B:3347:MET:N	2.51	0.44
1:C:399:MET:HE2	1:C:399:MET:N	2.33	0.44
1:D:1947:MET:HE3	1:D:1947:MET:HA	1.99	0.44
1:A:625:VAL:HG22	1:A:2132:ARG:HD3	1.99	0.44
1:A:4095:PHE:O	1:A:4099:VAL:HG23	2.18	0.44
1:B:399:MET:HE2	1:B:399:MET:N	2.33	0.44
1:B:655:MET:CE	1:B:834:VAL:HG12	2.48	0.44
1:B:2161:MET:SD	1:B:2161:MET:N	2.91	0.44
1:B:2298:LEU:HD13	1:B:2394:LEU:HA	1.98	0.44
1:C:1153:GLY:N	1:C:1183:LEU:O	2.51	0.44
1:C:1708:ILE:HG23	1:C:1828:THR:HG21	1.98	0.44
1:C:2402:ALA:O	1:C:2473:ARG:NH2	2.49	0.44
1:C:2714:GLU:OE1	1:C:2714:GLU:N	2.48	0.44
1:C:3176:LYS:O	1:C:3184:ASN:ND2	2.50	0.44
1:D:982:ASP:O	1:D:1055:ARG:NH2	2.51	0.44
1:D:1265:HIS:O	1:D:1288:LYS:NZ	2.39	0.44
1:D:3943:VAL:HG13	1:D:3977:MET:HE2	2.00	0.44
1:A:78:LEU:HD21	1:A:186:VAL:HG21	1.99	0.44
1:A:1021:GLN:OE1	1:A:1022:GLN:N	2.49	0.44
1:A:2251:GLU:OE1	1:A:2251:GLU:N	2.46	0.44
1:B:234:LEU:HD11	1:B:356:TYR:CE1	2.52	0.44
1:B:879:GLU:OE2	1:B:882:ARG:NH2	2.51	0.44
1:B:1988:PRO:CG	1:B:1991:ILE:HD12	2.47	0.44
1:B:2187:THR:HG23	1:B:2188:PHE:CD2	2.52	0.44
1:B:3176:LYS:O	1:B:3184:ASN:ND2	2.50	0.44
1:B:4095:PHE:O	1:B:4099:VAL:HG23	2.18	0.44
1:C:655:MET:CE	1:C:834:VAL:HG12	2.48	0.44
1:C:3170:LEU:HD23	1:C:3207:ILE:HG23	2.00	0.44
1:A:1730:MET:SD	1:A:1730:MET:N	2.84	0.44
1:A:3943:VAL:HG13	1:A:3977:MET:HE2	2.00	0.44
1:C:879:GLU:OE2	1:C:882:ARG:NH2	2.50	0.44
1:C:1114:ARG:NH1	1:C:1127:GLU:OE1	2.51	0.44
1:C:3346:ASP:OD1	1:C:3347:MET:N	2.51	0.44
1:C:3682:GLU:N	1:C:3682:GLU:OE1	2.49	0.44
1:D:1931:PHE:CE2	1:D:1935:LEU:HD21	2.53	0.44
1:D:2414:GLU:OE1	1:D:2414:GLU:N	2.47	0.44
1:D:3900:GLN:OE1	1:D:3903:ARG:NH2	2.50	0.44
1:A:1950:LEU:HD11	1:A:1960:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2394:LEU:O	1:A:2398:LEU:HD22	2.18	0.43
1:B:890:HIS:NE2	1:B:919:VAL:O	2.49	0.43
1:C:1463:ARG:O	1:C:1483:SER:OG	2.26	0.43
1:D:2251:GLU:OE1	1:D:2251:GLU:N	2.46	0.43
1:A:1931:PHE:CE2	1:A:1935:LEU:HD21	2.53	0.43
1:A:3900:GLN:OE1	1:A:3903:ARG:NH2	2.50	0.43
1:B:375:GLN:HG2	1:B:377:VAL:HG13	2.01	0.43
1:C:234:LEU:HD11	1:C:356:TYR:CE1	2.52	0.43
1:C:890:HIS:NE2	1:C:919:VAL:O	2.49	0.43
1:A:399:MET:HE2	1:A:399:MET:N	2.33	0.43
1:B:2271:CYS:O	1:B:2290:ASN:N	2.48	0.43
1:B:2405:MET:HE3	1:B:2408:ILE:HB	2.01	0.43
1:C:207:PHE:CE1	1:D:2324:ILE:HD13	2.54	0.43
1:A:606:ARG:NH2	1:A:1635:GLU:OE1	2.51	0.43
1:A:1114:ARG:NH1	1:A:1127:GLU:OE1	2.51	0.43
1:A:1708:ILE:HD11	1:A:1825:LEU:HA	2.00	0.43
1:A:2324:ILE:HD13	1:D:207:PHE:CE1	2.53	0.43
1:B:1189:GLU:OE1	1:B:1189:GLU:N	2.50	0.43
1:C:606:ARG:NH2	1:C:1635:GLU:OE1	2.52	0.43
1:C:1756:THR:N	1:C:1922:GLU:OE2	2.51	0.43
1:C:2394:LEU:O	1:C:2398:LEU:HD22	2.18	0.43
1:D:641:ASP:OD1	1:D:641:ASP:N	2.50	0.43
1:D:655:MET:CE	1:D:834:VAL:HG12	2.48	0.43
1:D:4095:PHE:O	1:D:4099:VAL:HG23	2.18	0.43
1:A:3170:LEU:HD23	1:A:3207:ILE:HG23	2.00	0.43
1:A:4181:GLU:OE1	1:A:4181:GLU:N	2.50	0.43
1:B:207:PHE:CE1	1:C:2324:ILE:HD13	2.54	0.43
1:B:642:LEU:O	1:B:642:LEU:HD13	2.19	0.43
1:B:1153:GLY:N	1:B:1183:LEU:O	2.51	0.43
1:D:606:ARG:NH2	1:D:1635:GLU:OE1	2.52	0.43
1:D:1114:ARG:NH1	1:D:1127:GLU:OE1	2.51	0.43
1:D:1988:PRO:CG	1:D:1991:ILE:HD12	2.47	0.43
2:H:67:MET:HG2	2:H:104:LEU:HD23	2.01	0.43
1:A:666:GLY:HA2	1:A:1012:ILE:HD13	2.01	0.43
1:A:1555:GLN:NE2	1:A:1557:GLU:OE2	2.48	0.43
1:A:2560:LEU:O	1:A:2565:ARG:NH1	2.52	0.43
1:A:3759:LYS:NZ	1:A:3833:GLU:OE2	2.51	0.43
1:B:565:LEU:HD11	1:B:1585:PRO:HG2	2.01	0.43
1:B:1114:ARG:NH1	1:B:1127:GLU:OE1	2.51	0.43
1:B:3854:GLN:NE2	1:B:3921:GLU:O	2.50	0.43
1:C:4050:ALA:O	1:C:4053:SER:OG	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2394:LEU:O	1:D:2398:LEU:HD22	2.18	0.43
1:D:3854:GLN:NE2	1:D:3921:GLU:O	2.50	0.43
1:A:982:ASP:O	1:A:1055:ARG:NH2	2.51	0.43
1:A:2337:GLU:OE1	1:A:2337:GLU:N	2.46	0.43
1:A:3333:VAL:HG21	1:A:3404:TYR:HB3	2.01	0.43
1:A:3891:TYR:OH	1:A:3898:ASP:OD1	2.33	0.43
1:B:606:ARG:NH2	1:B:1635:GLU:OE1	2.51	0.43
1:B:3170:LEU:HD23	1:B:3207:ILE:HG23	2.00	0.43
1:B:3649:GLU:OE1	1:B:3649:GLU:N	2.52	0.43
1:B:3943:VAL:HG13	1:B:3977:MET:HE2	2.00	0.43
1:C:271:ALA:N	1:C:491:GLU:OE2	2.46	0.43
1:C:1950:LEU:HD11	1:C:1960:LYS:NZ	2.33	0.43
1:D:399:MET:HE2	1:D:399:MET:N	2.33	0.43
1:D:565:LEU:HD11	1:D:1585:PRO:HG2	2.01	0.43
1:D:3759:LYS:NZ	1:D:3833:GLU:OE2	2.51	0.43
1:A:565:LEU:HD11	1:A:1585:PRO:HG2	2.01	0.43
1:A:2402:ALA:O	1:A:2473:ARG:NH2	2.50	0.43
1:B:982:ASP:O	1:B:1055:ARG:NH2	2.51	0.43
1:B:1650:GLU:OE1	1:B:1651:LEU:HD22	2.17	0.43
1:B:2337:GLU:OE1	1:B:2337:GLU:N	2.46	0.43
1:B:3333:VAL:HG21	1:B:3404:TYR:HB3	2.01	0.43
1:C:982:ASP:O	1:C:1055:ARG:NH2	2.51	0.43
1:C:4095:PHE:O	1:C:4099:VAL:HG23	2.18	0.43
1:D:1756:THR:N	1:D:1922:GLU:OE2	2.51	0.43
1:A:207:PHE:CE1	1:B:2324:ILE:HD13	2.54	0.43
1:A:3312:GLN:N	1:A:3312:GLN:OE1	2.52	0.43
1:B:666:GLY:HA2	1:B:1012:ILE:HD13	2.01	0.43
1:B:1266:GLU:OE1	1:B:1267:HIS:ND1	2.52	0.43
1:B:1555:GLN:NE2	1:B:1557:GLU:OE2	2.48	0.43
1:B:3312:GLN:OE1	1:B:3312:GLN:N	2.52	0.43
1:C:1708:ILE:HD11	1:C:1825:LEU:HA	2.01	0.43
1:C:2161:MET:HE3	1:C:2166:MET:SD	2.58	0.43
1:D:3628:ILE:HD12	1:D:3629:GLU:N	2.34	0.43
1:A:1756:THR:N	1:A:1922:GLU:OE2	2.51	0.43
1:A:2714:GLU:OE1	1:A:2714:GLU:N	2.48	0.43
1:A:2946:SER:O	1:A:2949:LYS:N	2.52	0.43
1:B:1931:PHE:CE2	1:B:1935:LEU:HD21	2.53	0.43
1:C:565:LEU:HD11	1:C:1585:PRO:HG2	2.01	0.43
1:C:666:GLY:HA2	1:C:1012:ILE:HD13	2.01	0.43
1:C:2435:ILE:O	1:C:2464:LYS:NZ	2.40	0.43
1:C:3166:PRO:HD2	1:C:3167:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1153:GLY:N	1:D:1183:LEU:O	2.51	0.43
1:D:1809:ASP:OD1	1:D:1809:ASP:N	2.52	0.43
1:B:1950:LEU:HD11	1:B:1960:LYS:NZ	2.33	0.42
1:C:1931:PHE:CE2	1:C:1935:LEU:HD21	2.53	0.42
1:C:3333:VAL:HG21	1:C:3404:TYR:HB3	2.01	0.42
1:C:3943:VAL:HG13	1:C:3977:MET:HE2	2.00	0.42
1:D:2171:MET:HE2	1:D:2216:HIS:HB3	2.01	0.42
1:D:3176:LYS:O	1:D:3184:ASN:ND2	2.50	0.42
1:B:1809:ASP:N	1:B:1809:ASP:OD1	2.52	0.42
1:D:375:GLN:HG2	1:D:377:VAL:HG13	2.01	0.42
1:D:1189:GLU:OE1	1:D:1189:GLU:N	2.50	0.42
1:D:3312:GLN:OE1	1:D:3312:GLN:N	2.52	0.42
2:H:25:VAL:HG12	2:H:104:LEU:HD22	2.01	0.42
1:A:116:GLY:N	1:A:162:ILE:O	2.46	0.42
1:A:375:GLN:HG2	1:A:377:VAL:HG13	2.01	0.42
1:A:2405:MET:HE3	1:A:2408:ILE:HB	2.00	0.42
1:B:363:ILE:HD12	1:B:363:ILE:N	2.35	0.42
1:C:642:LEU:HD13	1:C:642:LEU:O	2.19	0.42
1:C:2171:MET:HE2	1:C:2216:HIS:HB3	2.01	0.42
1:C:2569:GLU:OE1	1:C:2570:VAL:HG13	2.18	0.42
1:D:642:LEU:HD13	1:D:642:LEU:O	2.19	0.42
1:D:1139:GLY:O	1:D:1155:SER:OG	2.19	0.42
1:D:1708:ILE:HD11	1:D:1825:LEU:HA	2.01	0.42
1:D:3170:LEU:HD23	1:D:3207:ILE:HG23	2.00	0.42
2:G:67:MET:HG2	2:G:104:LEU:HD23	2.01	0.42
1:A:1189:GLU:OE1	1:A:1189:GLU:N	2.50	0.42
1:A:1266:GLU:OE1	1:A:1267:HIS:ND1	2.52	0.42
1:B:3961:SER:O	1:B:3961:SER:OG	2.37	0.42
1:B:4089:PRO:O	1:B:4093:ILE:HD12	2.20	0.42
1:C:1266:GLU:OE1	1:C:1267:HIS:ND1	2.52	0.42
1:C:1730:MET:SD	1:C:1730:MET:N	2.84	0.42
1:C:4089:PRO:O	1:C:4093:ILE:HD12	2.20	0.42
1:D:38:ALA:HB1	1:D:64:ILE:HG22	2.01	0.42
1:D:744:PRO:O	1:D:745:ASN:ND2	2.40	0.42
1:D:1950:LEU:HD11	1:D:1960:LYS:NZ	2.34	0.42
1:D:3333:VAL:HG21	1:D:3404:TYR:HB3	2.01	0.42
1:D:3661:ASP:OD1	1:D:3661:ASP:N	2.53	0.42
1:D:1266:GLU:OE1	1:D:1267:HIS:ND1	2.52	0.42
1:D:1574:SER:OG	1:D:1575:GLU:OE1	2.27	0.42
1:D:2405:MET:HE3	1:D:2408:ILE:HB	2.01	0.42
2:J:67:MET:HG2	2:J:104:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ALA:HB1	1:A:64:ILE:HG22	2.01	0.42
1:A:1809:ASP:OD1	1:A:1809:ASP:N	2.52	0.42
1:B:655:MET:HE3	1:B:834:VAL:HG12	2.02	0.42
1:B:2801:ASN:OD1	1:B:2802:ARG:N	2.53	0.42
1:B:3628:ILE:HD12	1:B:3629:GLU:N	2.34	0.42
1:D:2801:ASN:OD1	1:D:2802:ARG:N	2.53	0.42
1:D:4089:PRO:O	1:D:4093:ILE:HD12	2.20	0.42
2:I:67:MET:HG2	2:I:104:LEU:HD23	2.01	0.42
1:A:232:ASP:OD2	1:A:356:TYR:OH	2.38	0.42
1:B:4883:MET:HE1	1:B:4888:PHE:HD1	1.85	0.42
1:C:1031:ARG:NH1	1:C:1038:LEU:HD22	2.34	0.42
1:C:1139:GLY:O	1:C:1155:SER:OG	2.19	0.42
1:C:3661:ASP:OD1	1:C:3661:ASP:N	2.53	0.42
1:A:3628:ILE:HD12	1:A:3629:GLU:N	2.34	0.42
1:C:3628:ILE:HD12	1:C:3629:GLU:N	2.34	0.42
1:D:666:GLY:HA2	1:D:1012:ILE:HD13	2.01	0.42
1:D:3667:ILE:HG21	1:D:3733:ARG:O	2.20	0.42
1:B:4616:ILE:HG12	1:B:4665:ILE:HD12	2.02	0.42
1:C:655:MET:HE3	1:C:834:VAL:HG12	2.02	0.42
1:C:986:ILE:O	1:C:1055:ARG:NH1	2.53	0.42
1:C:1215:MET:HE3	1:C:1215:MET:HA	2.02	0.42
1:C:2801:ASN:OD1	1:C:2802:ARG:N	2.53	0.42
1:C:3649:GLU:OE1	1:C:3649:GLU:N	2.52	0.42
1:D:19:GLU:N	1:D:218:SER:O	2.48	0.42
1:A:642:LEU:HD13	1:A:642:LEU:O	2.19	0.42
1:B:130:LEU:HA	1:B:149:LEU:HD23	2.02	0.42
1:B:1031:ARG:NH1	1:B:1038:LEU:HD22	2.34	0.42
1:C:4883:MET:HE1	1:C:4888:PHE:HD1	1.84	0.42
1:D:364:GLN:NE2	1:D:369:GLY:O	2.49	0.42
1:D:2128:LEU:HD21	1:D:2137:GLU:CB	2.50	0.42
1:A:4089:PRO:O	1:A:4093:ILE:HD12	2.20	0.41
1:A:4616:ILE:HG12	1:A:4665:ILE:HD12	2.02	0.41
1:B:131:CYS:SG	1:B:150:GLN:NE2	2.91	0.41
1:B:2171:MET:HE2	1:B:2216:HIS:HB3	2.01	0.41
1:C:3269:SER:OG	1:C:3310:LYS:NZ	2.44	0.41
1:A:2171:MET:HE2	1:A:2216:HIS:HB3	2.01	0.41
1:A:2801:ASN:OD1	1:A:2802:ARG:N	2.53	0.41
1:B:1276:THR:N	1:B:1279:SER:O	2.53	0.41
1:B:2175:VAL:HG22	1:B:2219:TYR:CE2	2.55	0.41
1:B:3166:PRO:HD2	1:B:3167:ILE:HD12	2.01	0.41
1:B:4050:ALA:O	1:B:4053:SER:OG	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:ASN:ND2	1:C:745:ASN:O	2.54	0.41
1:C:2502:ASP:OD2	1:C:2553:ARG:NH1	2.53	0.41
1:C:3667:ILE:HG21	1:C:3733:ARG:O	2.20	0.41
1:D:2560:LEU:O	1:D:2565:ARG:NH1	2.52	0.41
1:A:364:GLN:NE2	1:A:369:GLY:O	2.49	0.41
1:A:1031:ARG:NH1	1:A:1038:LEU:HD22	2.34	0.41
1:A:1276:THR:N	1:A:1279:SER:O	2.53	0.41
1:A:3661:ASP:OD1	1:A:3661:ASP:N	2.53	0.41
1:B:38:ALA:HB1	1:B:64:ILE:HG22	2.01	0.41
1:B:986:ILE:O	1:B:1055:ARG:NH1	2.53	0.41
1:C:1168:MET:N	1:C:1168:MET:SD	2.86	0.41
1:C:1189:GLU:OE1	1:C:1189:GLU:N	2.50	0.41
1:D:363:ILE:HD12	1:D:363:ILE:N	2.35	0.41
1:D:4883:MET:HE1	1:D:4888:PHE:HD1	1.85	0.41
1:A:745:ASN:ND2	1:A:745:ASN:O	2.54	0.41
1:A:2502:ASP:OD2	1:A:2553:ARG:NH1	2.53	0.41
1:A:3176:LYS:O	1:A:3184:ASN:ND2	2.50	0.41
1:A:4883:MET:HE1	1:A:4888:PHE:HD1	1.85	0.41
1:B:2502:ASP:OD2	1:B:2553:ARG:NH1	2.53	0.41
1:C:1555:GLN:NE2	1:C:1557:GLU:OE2	2.48	0.41
1:C:1809:ASP:OD1	1:C:1809:ASP:N	2.52	0.41
1:D:745:ASN:ND2	1:D:745:ASN:O	2.54	0.41
1:D:986:ILE:O	1:D:1055:ARG:NH1	2.53	0.41
1:D:1031:ARG:NH1	1:D:1038:LEU:HD22	2.34	0.41
1:A:130:LEU:HA	1:A:149:LEU:HD23	2.02	0.41
1:A:2233:MET:HE3	1:A:2233:MET:HA	2.03	0.41
1:A:3166:PRO:HD2	1:A:3167:ILE:HD12	2.01	0.41
1:B:116:GLY:N	1:B:162:ILE:O	2.47	0.41
1:B:3667:ILE:HG21	1:B:3733:ARG:O	2.20	0.41
1:D:241:MET:SD	1:D:242:ASP:N	2.94	0.41
1:D:2502:ASP:OD2	1:D:2553:ARG:NH1	2.53	0.41
1:D:2946:SER:O	1:D:2949:LYS:N	2.52	0.41
2:G:25:VAL:HG12	2:G:104:LEU:HD22	2.02	0.41
1:A:186:VAL:O	1:B:2417:ARG:NH1	2.53	0.41
1:A:363:ILE:N	1:A:363:ILE:HD12	2.35	0.41
1:A:1792:THR:HG21	1:A:1825:LEU:CD2	2.51	0.41
1:A:4614:LEU:HD13	1:A:4614:LEU:O	2.21	0.41
1:B:1276:THR:OG1	1:B:1278:ASP:OD1	2.34	0.41
1:B:4087:HIS:O	1:B:4091:LYS:N	2.44	0.41
1:C:54:ASN:OD1	1:C:57:ASN:ND2	2.53	0.41
1:C:2946:SER:O	1:C:2949:LYS:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3312:GLN:N	1:C:3312:GLN:OE1	2.52	0.41
1:C:4616:ILE:HG12	1:C:4665:ILE:HD12	2.02	0.41
1:D:655:MET:HE3	1:D:834:VAL:HG12	2.01	0.41
2:I:25:VAL:HG12	2:I:104:LEU:HD22	2.01	0.41
1:A:1267:HIS:O	1:A:1288:LYS:N	2.47	0.41
1:C:1565:MET:HE1	1:C:1579:PRO:HA	2.03	0.41
1:D:1792:THR:HG21	1:D:1825:LEU:CD2	2.51	0.41
1:A:54:ASN:OD1	1:A:57:ASN:ND2	2.54	0.41
1:A:241:MET:SD	1:A:242:ASP:N	2.94	0.41
1:A:655:MET:HE3	1:A:834:VAL:HG12	2.02	0.41
1:A:1215:MET:HA	1:A:1215:MET:HE3	2.02	0.41
1:A:1283:LEU:HD23	1:A:1589:VAL:HG13	2.03	0.41
1:A:3667:ILE:HG21	1:A:3733:ARG:O	2.20	0.41
1:C:241:MET:SD	1:C:242:ASP:N	2.94	0.41
1:D:130:LEU:HA	1:D:149:LEU:HD23	2.03	0.41
1:D:1276:THR:N	1:D:1279:SER:O	2.54	0.41
1:D:4614:LEU:HD13	1:D:4614:LEU:O	2.21	0.41
1:A:986:ILE:O	1:A:1055:ARG:NH1	2.53	0.41
1:A:1742:ASP:OD2	1:A:1744:ASN:ND2	2.54	0.41
1:A:2972:GLN:OE1	1:A:2976:ASN:ND2	2.54	0.41
1:A:3376:VAL:HG12	1:A:3383:TRP:CZ3	2.56	0.41
1:B:54:ASN:OD1	1:B:57:ASN:ND2	2.53	0.41
1:B:186:VAL:O	1:C:2417:ARG:NH1	2.53	0.41
1:B:241:MET:SD	1:B:242:ASP:N	2.94	0.41
1:B:1283:LEU:HD23	1:B:1589:VAL:HG13	2.03	0.41
1:B:1565:MET:HE1	1:B:1579:PRO:HA	2.03	0.41
1:B:2078:GLU:OE1	1:B:2078:GLU:N	2.44	0.41
1:B:2233:MET:HE3	1:B:2233:MET:HA	2.02	0.41
1:B:2399:GLY:O	1:B:2473:ARG:NE	2.52	0.41
1:B:4614:LEU:HD13	1:B:4614:LEU:O	2.21	0.41
1:C:130:LEU:HA	1:C:149:LEU:HD23	2.03	0.41
1:C:1017:THR:C	1:C:1032:LEU:HD12	2.46	0.41
1:C:1022:GLN:N	1:C:1022:GLN:OE1	2.54	0.41
1:C:1276:THR:N	1:C:1279:SER:O	2.53	0.41
1:C:2405:MET:HE3	1:C:2408:ILE:HB	2.03	0.41
1:D:676:GLU:OE1	1:D:812:LYS:N	2.47	0.41
1:D:1017:THR:C	1:D:1032:LEU:HD12	2.46	0.41
1:D:2507:SER:HG	1:D:2559:SER:HG	1.61	0.41
1:D:3649:GLU:OE1	1:D:3649:GLU:N	2.52	0.41
1:D:4616:ILE:HG12	1:D:4665:ILE:HD12	2.02	0.41
1:A:1153:GLY:N	1:A:1183:LEU:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4653:MET:HE1	1:A:4665:ILE:HB	2.03	0.41
1:B:3376:VAL:HG12	1:B:3383:TRP:CZ3	2.57	0.41
1:C:116:GLY:N	1:C:162:ILE:O	2.46	0.41
1:C:232:ASP:OD2	1:C:356:TYR:OH	2.39	0.41
1:C:2236:SER:N	1:C:2240:ASP:OD2	2.54	0.41
1:D:2233:MET:HA	1:D:2233:MET:HE3	2.03	0.41
1:D:4653:MET:HE1	1:D:4665:ILE:HB	2.03	0.41
2:J:25:VAL:HG12	2:J:104:LEU:HD22	2.02	0.41
1:A:2236:SER:N	1:A:2240:ASP:OD2	2.55	0.40
1:A:2423:ARG:O	1:A:2475:TYR:OH	2.30	0.40
1:A:3649:GLU:OE1	1:A:3649:GLU:N	2.52	0.40
1:B:19:GLU:N	1:B:218:SER:O	2.48	0.40
1:B:1017:THR:C	1:B:1032:LEU:HD12	2.46	0.40
1:B:1988:PRO:HG2	1:B:1991:ILE:HD12	2.03	0.40
1:C:87:GLU:OE1	1:C:87:GLU:N	2.42	0.40
1:C:2656:TYR:OH	1:C:2658:GLN:OE1	2.33	0.40
1:C:2972:GLN:OE1	1:C:2976:ASN:ND2	2.54	0.40
1:C:3103:MET:O	1:C:3106:SER:OG	2.33	0.40
1:D:232:ASP:OD2	1:D:356:TYR:OH	2.38	0.40
1:D:2972:GLN:OE1	1:D:2976:ASN:ND2	2.54	0.40
1:D:3263:CYS:SG	1:D:3264:CYS:N	2.80	0.40
1:A:3667:ILE:HG23	1:A:3738:MET:HE3	2.03	0.40
1:B:2946:SER:O	1:B:2949:LYS:N	2.52	0.40
1:C:3667:ILE:HG23	1:C:3738:MET:HE3	2.03	0.40
1:C:4883:MET:HE2	1:C:4883:MET:HA	2.04	0.40
1:A:1769:PHE:CE2	2:G:91:VAL:HG21	2.57	0.40
1:A:2385:ASN:ND2	1:A:2458:GLY:O	2.55	0.40
1:B:232:ASP:OD2	1:B:356:TYR:OH	2.38	0.40
1:B:3943:VAL:HG11	1:B:4001:MET:CE	2.52	0.40
1:C:2118:LEU:HD22	1:C:2148:ILE:CD1	2.51	0.40
1:D:3166:PRO:HD2	1:D:3167:ILE:HD12	2.01	0.40
1:B:2478:GLU:N	1:B:2478:GLU:OE1	2.55	0.40
1:B:4653:MET:HE1	1:B:4665:ILE:HB	2.03	0.40
1:C:3943:VAL:HG11	1:C:4001:MET:CE	2.52	0.40
1:D:1769:PHE:CE2	2:J:91:VAL:HG21	2.57	0.40
1:D:2492:LEU:HD23	1:D:2547:LEU:HD22	2.04	0.40
1:A:337:LYS:NZ	1:A:396:GLU:OE2	2.36	0.40
1:A:1565:MET:HE1	1:A:1579:PRO:HA	2.03	0.40
1:A:2118:LEU:HD22	1:A:2148:ILE:CD1	2.51	0.40
1:B:364:GLN:NE2	1:B:369:GLY:O	2.50	0.40
1:B:1769:PHE:CE2	2:H:91:VAL:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3667:ILE:HG23	1:B:3738:MET:HE3	2.03	0.40
1:C:38:ALA:HB1	1:C:64:ILE:HG22	2.02	0.40
1:C:1283:LEU:HD23	1:C:1589:VAL:HG13	2.03	0.40
1:C:1769:PHE:CE2	2:I:91:VAL:HG21	2.57	0.40
1:C:1792:THR:HG21	1:C:1825:LEU:CD2	2.51	0.40
1:C:2233:MET:HE3	1:C:2233:MET:HA	2.02	0.40
1:D:1215:MET:HE3	1:D:1215:MET:HA	2.02	0.40
1:D:2271:CYS:O	1:D:2290:ASN:N	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4194/4966 (84%)	4028 (96%)	166 (4%)	0	100	100
1	B	4194/4966 (84%)	4027 (96%)	167 (4%)	0	100	100
1	C	4194/4966 (84%)	4027 (96%)	167 (4%)	0	100	100
1	D	4194/4966 (84%)	4029 (96%)	165 (4%)	0	100	100
2	G	105/176 (60%)	96 (91%)	9 (9%)	0	100	100
2	H	105/176 (60%)	96 (91%)	9 (9%)	0	100	100
2	I	105/176 (60%)	96 (91%)	9 (9%)	0	100	100
2	J	105/176 (60%)	96 (91%)	9 (9%)	0	100	100
All	All	17196/20568 (84%)	16495 (96%)	701 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3696/4355 (85%)	3626 (98%)	70 (2%)	50 73
1	B	3696/4355 (85%)	3627 (98%)	69 (2%)	50 73
1	C	3696/4355 (85%)	3626 (98%)	70 (2%)	50 73
1	D	3696/4355 (85%)	3629 (98%)	67 (2%)	51 74
2	G	88/140 (63%)	82 (93%)	6 (7%)	14 31
2	H	88/140 (63%)	81 (92%)	7 (8%)	11 24
2	I	88/140 (63%)	82 (93%)	6 (7%)	14 31
2	J	88/140 (63%)	81 (92%)	7 (8%)	11 24
All	All	15136/17980 (84%)	14834 (98%)	302 (2%)	48 72

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	110	HIS
1	A	114	LEU
1	A	117	HIS
1	A	185	SER
1	A	213	SER
1	A	236	LEU
1	A	246	THR
1	A	332	ARG
1	A	347	ASP
1	A	555	LEU
1	A	745	ASN
1	A	748	LEU
1	A	822	CYS
1	A	918	LEU
1	A	1029	ASN
1	A	1156	TRP
1	A	1251	LEU
1	A	1306	MET

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Mol	Chain	Res	Type
1	A	1429	SER
1	A	1561	ILE
1	A	1598	SER
1	A	1642	ILE
1	A	1721	MET
1	A	1754	LEU
1	A	1895	MET
1	A	1939	GLN
1	A	1948	GLN
1	A	1966	SER
1	A	1985	CYS
1	A	2128	LEU
1	A	2160	LEU
1	A	2166	MET
1	A	2221	LEU
1	A	2279	LEU
1	A	2430	ASP
1	A	2519	LEU
1	A	2527	LEU
1	A	2569	GLU
1	A	2572	LEU
1	A	2574	SER
1	A	2576	CYS
1	A	2583	MET
1	A	2611	ASN
1	A	2668	LEU
1	A	2707	THR
1	A	2721	ASN
1	A	2746	TYR
1	A	2777	SER
1	A	2884	ASP
1	A	2974	PHE
1	A	3027	SER
1	A	3047	THR
1	A	3272	MET
1	A	3372	LEU
1	A	3388	ASN
1	A	3607	LEU
1	A	3697	SER
1	A	3958	SER
1	A	3961	SER
1	A	4043	SER

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Mol	Chain	Res	Type
1	A	4117	PHE
1	A	4140	SER
1	A	4147	VAL
1	A	4152	SER
1	A	4500	MET
1	A	4518	TYR
1	A	4668	LEU
1	A	4749	PHE
1	A	4862	GLN
1	B	52	THR
1	B	110	HIS
1	B	114	LEU
1	B	117	HIS
1	B	185	SER
1	B	213	SER
1	B	236	LEU
1	B	246	THR
1	B	332	ARG
1	B	347	ASP
1	B	555	LEU
1	B	745	ASN
1	B	748	LEU
1	B	822	CYS
1	B	1029	ASN
1	B	1156	TRP
1	B	1180	GLU
1	B	1306	MET
1	B	1429	SER
1	B	1561	ILE
1	B	1598	SER
1	B	1642	ILE
1	B	1721	MET
1	B	1754	LEU
1	B	1895	MET
1	B	1939	GLN
1	B	1948	GLN
1	B	1966	SER
1	B	1985	CYS
1	B	2128	LEU
1	B	2160	LEU
1	B	2221	LEU
1	B	2279	LEU

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Mol	Chain	Res	Type
1	B	2430	ASP
1	B	2519	LEU
1	B	2527	LEU
1	B	2569	GLU
1	B	2572	LEU
1	B	2574	SER
1	B	2576	CYS
1	B	2583	MET
1	B	2611	ASN
1	B	2668	LEU
1	B	2707	THR
1	B	2721	ASN
1	B	2746	TYR
1	B	2777	SER
1	B	2884	ASP
1	B	2974	PHE
1	B	3027	SER
1	B	3047	THR
1	B	3245	MET
1	B	3272	MET
1	B	3372	LEU
1	B	3388	ASN
1	B	3607	LEU
1	B	3697	SER
1	B	3958	SER
1	B	3961	SER
1	B	3967	LEU
1	B	4043	SER
1	B	4117	PHE
1	B	4140	SER
1	B	4147	VAL
1	B	4152	SER
1	B	4500	MET
1	B	4518	TYR
1	B	4668	LEU
1	B	4862	GLN
1	C	52	THR
1	C	110	HIS
1	C	114	LEU
1	C	117	HIS
1	C	124	SER
1	C	185	SER

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Mol	Chain	Res	Type
1	C	213	SER
1	C	236	LEU
1	C	246	THR
1	C	332	ARG
1	C	347	ASP
1	C	363	ILE
1	C	555	LEU
1	C	745	ASN
1	C	748	LEU
1	C	822	CYS
1	C	1029	ASN
1	C	1156	TRP
1	C	1306	MET
1	C	1429	SER
1	C	1561	ILE
1	C	1598	SER
1	C	1642	ILE
1	C	1721	MET
1	C	1754	LEU
1	C	1895	MET
1	C	1939	GLN
1	C	1948	GLN
1	C	1966	SER
1	C	1985	CYS
1	C	2128	LEU
1	C	2160	LEU
1	C	2166	MET
1	C	2221	LEU
1	C	2279	LEU
1	C	2430	ASP
1	C	2519	LEU
1	C	2527	LEU
1	C	2569	GLU
1	C	2572	LEU
1	C	2574	SER
1	C	2576	CYS
1	C	2583	MET
1	C	2611	ASN
1	C	2668	LEU
1	C	2707	THR
1	C	2721	ASN
1	C	2746	TYR

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Mol	Chain	Res	Type
1	C	2777	SER
1	C	2884	ASP
1	C	2974	PHE
1	C	3027	SER
1	C	3047	THR
1	C	3272	MET
1	C	3372	LEU
1	C	3388	ASN
1	C	3607	LEU
1	C	3697	SER
1	C	3958	SER
1	C	3961	SER
1	C	3967	LEU
1	C	4043	SER
1	C	4117	PHE
1	C	4140	SER
1	C	4147	VAL
1	C	4152	SER
1	C	4500	MET
1	C	4518	TYR
1	C	4668	LEU
1	C	4862	GLN
1	D	52	THR
1	D	110	HIS
1	D	114	LEU
1	D	117	HIS
1	D	185	SER
1	D	213	SER
1	D	236	LEU
1	D	246	THR
1	D	332	ARG
1	D	347	ASP
1	D	555	LEU
1	D	745	ASN
1	D	748	LEU
1	D	822	CYS
1	D	918	LEU
1	D	1029	ASN
1	D	1156	TRP
1	D	1251	LEU
1	D	1306	MET
1	D	1429	SER

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Mol	Chain	Res	Type
1	D	1561	ILE
1	D	1598	SER
1	D	1642	ILE
1	D	1721	MET
1	D	1754	LEU
1	D	1895	MET
1	D	1939	GLN
1	D	1948	GLN
1	D	1966	SER
1	D	1985	CYS
1	D	2160	LEU
1	D	2166	MET
1	D	2221	LEU
1	D	2279	LEU
1	D	2430	ASP
1	D	2519	LEU
1	D	2527	LEU
1	D	2569	GLU
1	D	2572	LEU
1	D	2574	SER
1	D	2576	CYS
1	D	2583	MET
1	D	2611	ASN
1	D	2707	THR
1	D	2721	ASN
1	D	2746	TYR
1	D	2777	SER
1	D	2884	ASP
1	D	2974	PHE
1	D	3027	SER
1	D	3047	THR
1	D	3272	MET
1	D	3372	LEU
1	D	3388	ASN
1	D	3607	LEU
1	D	3697	SER
1	D	3958	SER
1	D	3961	SER
1	D	4043	SER
1	D	4117	PHE
1	D	4140	SER
1	D	4147	VAL

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Mol	Chain	Res	Type
1	D	4152	SER
1	D	4500	MET
1	D	4518	TYR
1	D	4668	LEU
1	D	4862	GLN
2	G	18	LYS
2	G	25	VAL
2	G	26	HIS
2	G	39	SER
2	G	42	ASP
2	G	104	LEU
2	H	18	LYS
2	H	25	VAL
2	H	26	HIS
2	H	30	MET
2	H	39	SER
2	H	42	ASP
2	H	104	LEU
2	I	18	LYS
2	I	25	VAL
2	I	26	HIS
2	I	39	SER
2	I	42	ASP
2	I	104	LEU
2	J	18	LYS
2	J	25	VAL
2	J	26	HIS
2	J	30	MET
2	J	39	SER
2	J	42	ASP
2	J	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	HIS
1	A	1026	ASN
1	A	1257	GLN
1	A	1774	ASN
1	A	2088	HIS
1	A	2210	GLN
1	A	2223	ASN

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Mol	Chain	Res	Type
1	A	3178	ASN
1	A	3303	GLN
1	A	4170	GLN
1	A	4932	HIS
1	B	472	HIS
1	B	1026	ASN
1	B	1149	ASN
1	B	1547	GLN
1	B	1774	ASN
1	B	2088	HIS
1	B	2210	GLN
1	B	2440	GLN
1	B	3178	ASN
1	B	3303	GLN
1	B	4170	GLN
1	B	4932	HIS
1	C	472	HIS
1	C	1026	ASN
1	C	1149	ASN
1	C	1257	GLN
1	C	1547	GLN
1	C	2088	HIS
1	C	2223	ASN
1	C	2317	ASN
1	C	3178	ASN
1	C	3303	GLN
1	C	4170	GLN
1	C	4932	HIS
1	D	57	ASN
1	D	472	HIS
1	D	1026	ASN
1	D	1149	ASN
1	D	1257	GLN
1	D	1774	ASN
1	D	2317	ASN
1	D	3178	ASN
1	D	3303	GLN
1	D	3811	ASN
1	D	4170	GLN
1	D	4932	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

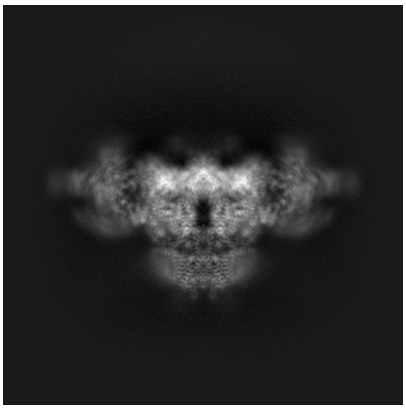
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80684. These allow visual inspection of the internal detail of the map and identification of artifacts.

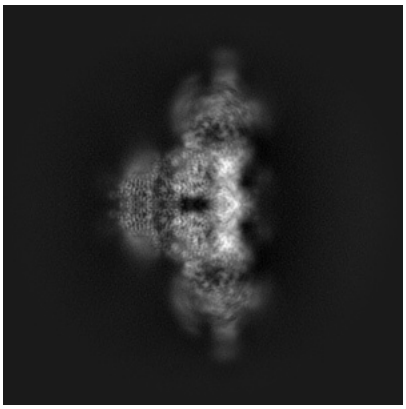
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

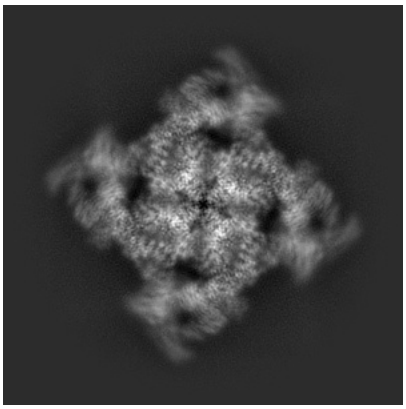
6.1.1 Primary map



X

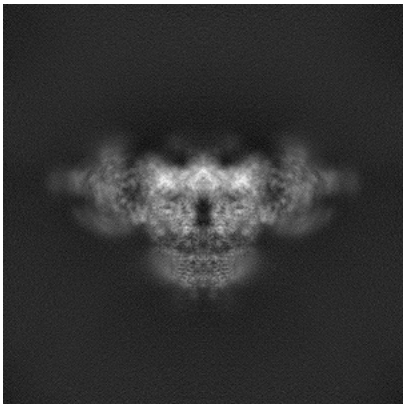


Y

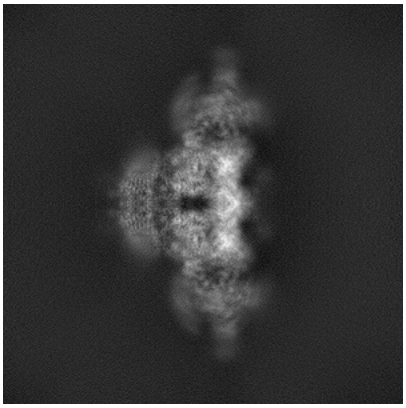


Z

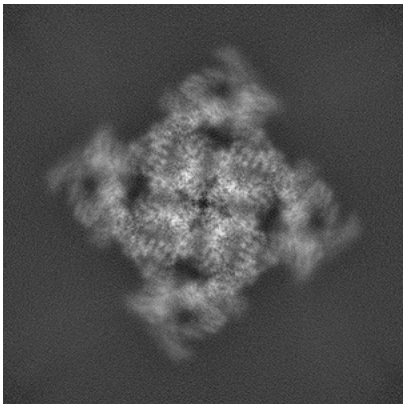
6.1.2 Raw map



X



Y



Z

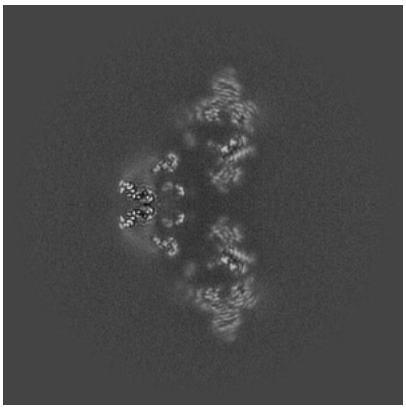
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

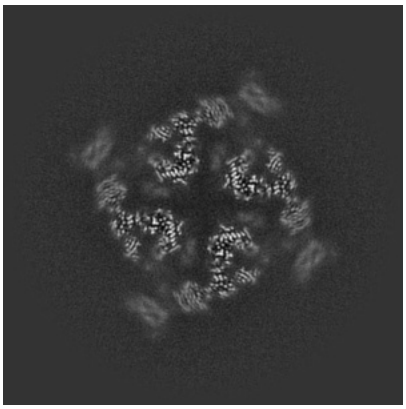
6.2.1 Primary map



X Index: 256



Y Index: 256

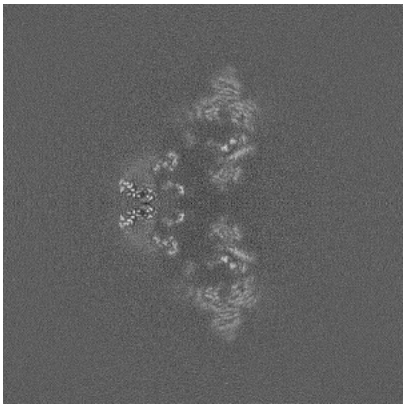


Z Index: 256

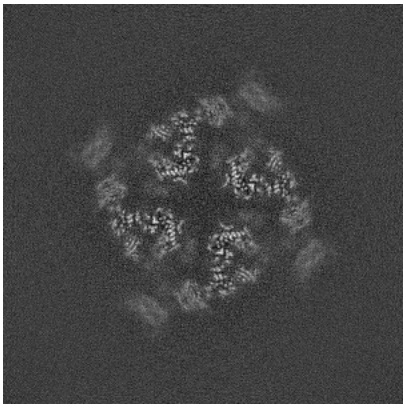
6.2.2 Raw map



X Index: 256



Y Index: 256

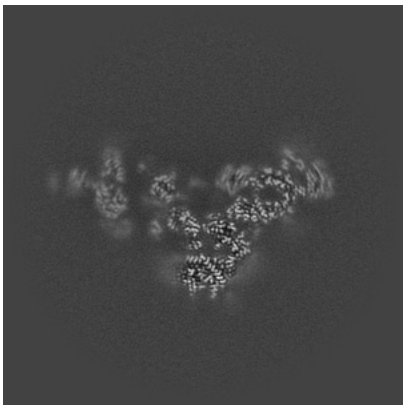


Z Index: 256

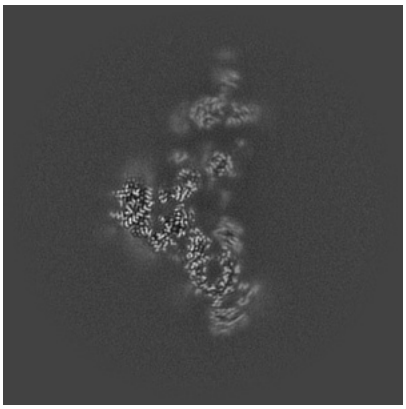
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

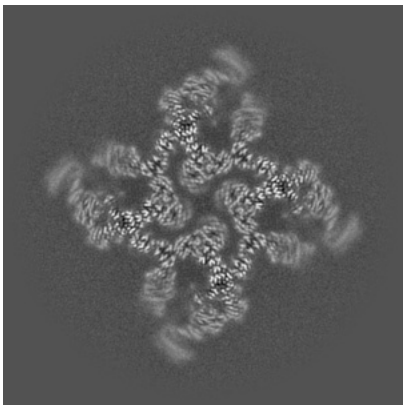
6.3.1 Primary map



X Index: 240

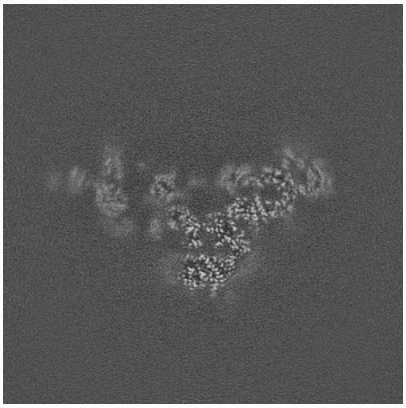


Y Index: 240



Z Index: 285

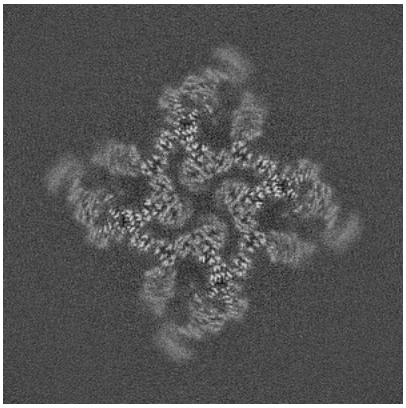
6.3.2 Raw map



X Index: 239



Y Index: 273



Z Index: 285

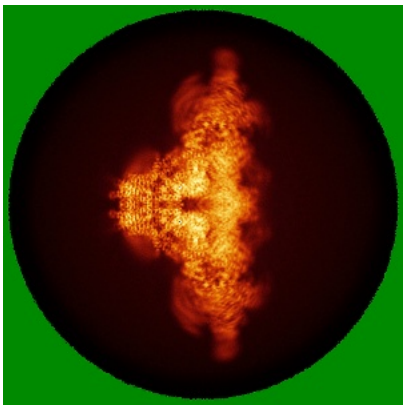
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

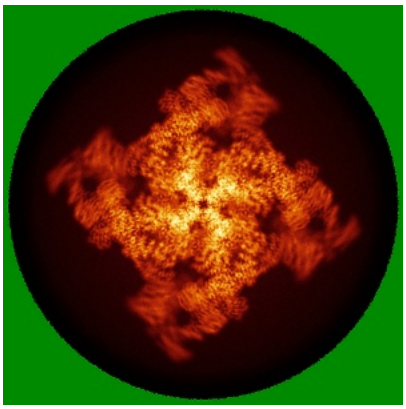
6.4.1 Primary map



X

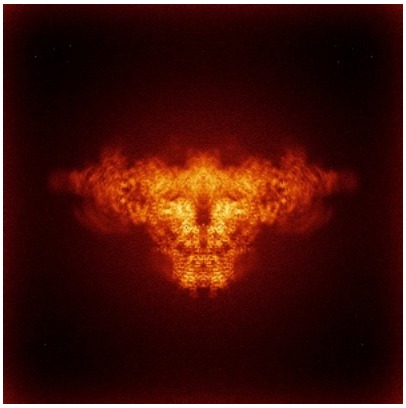


Y

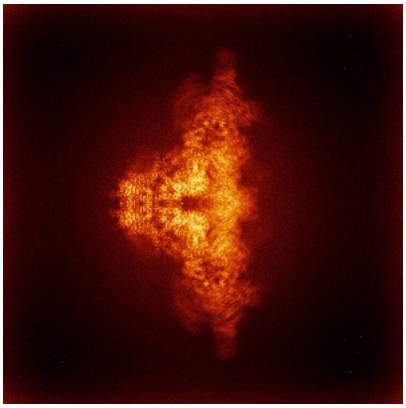


Z

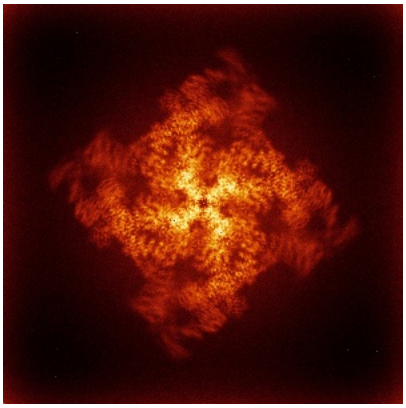
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

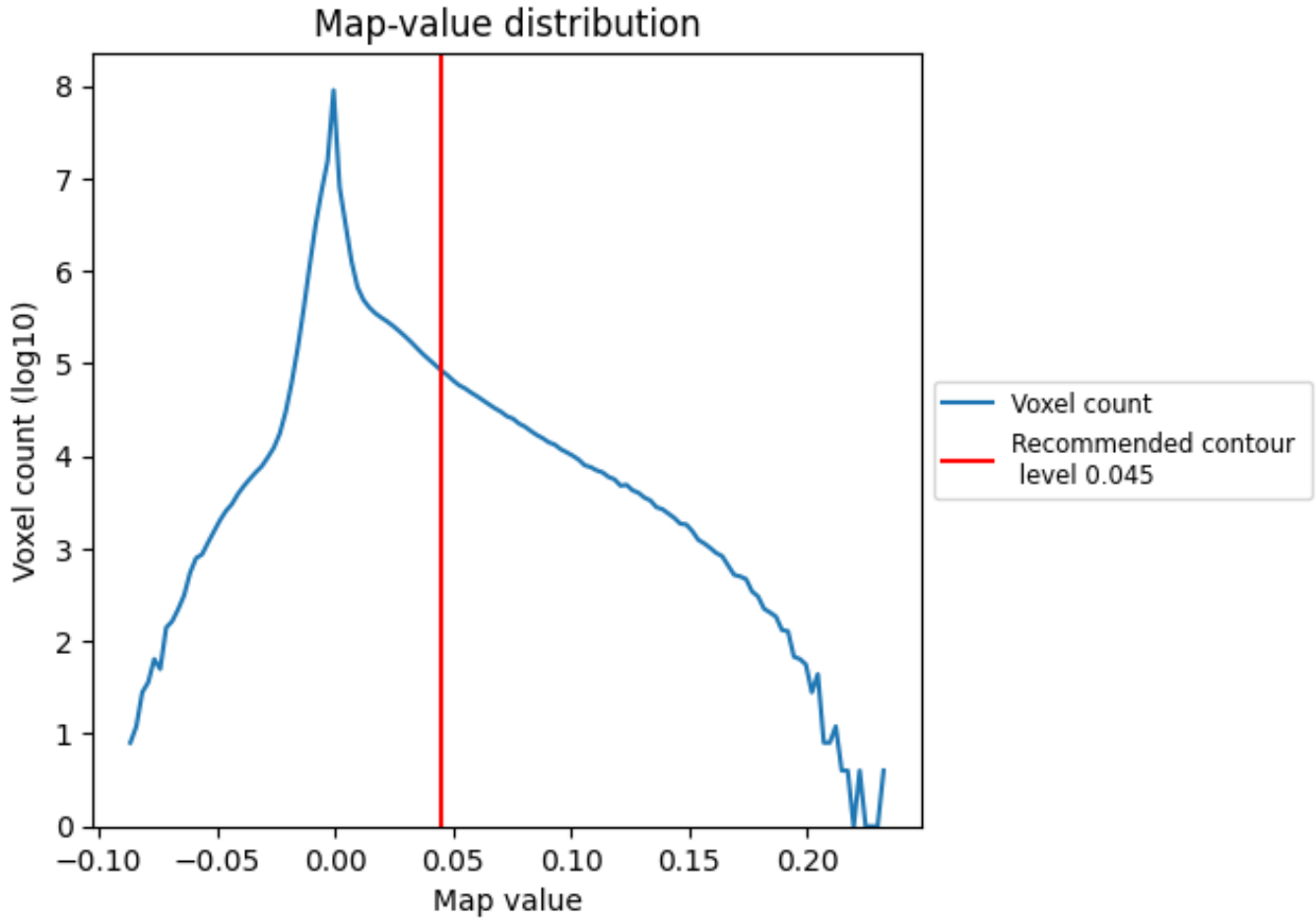
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

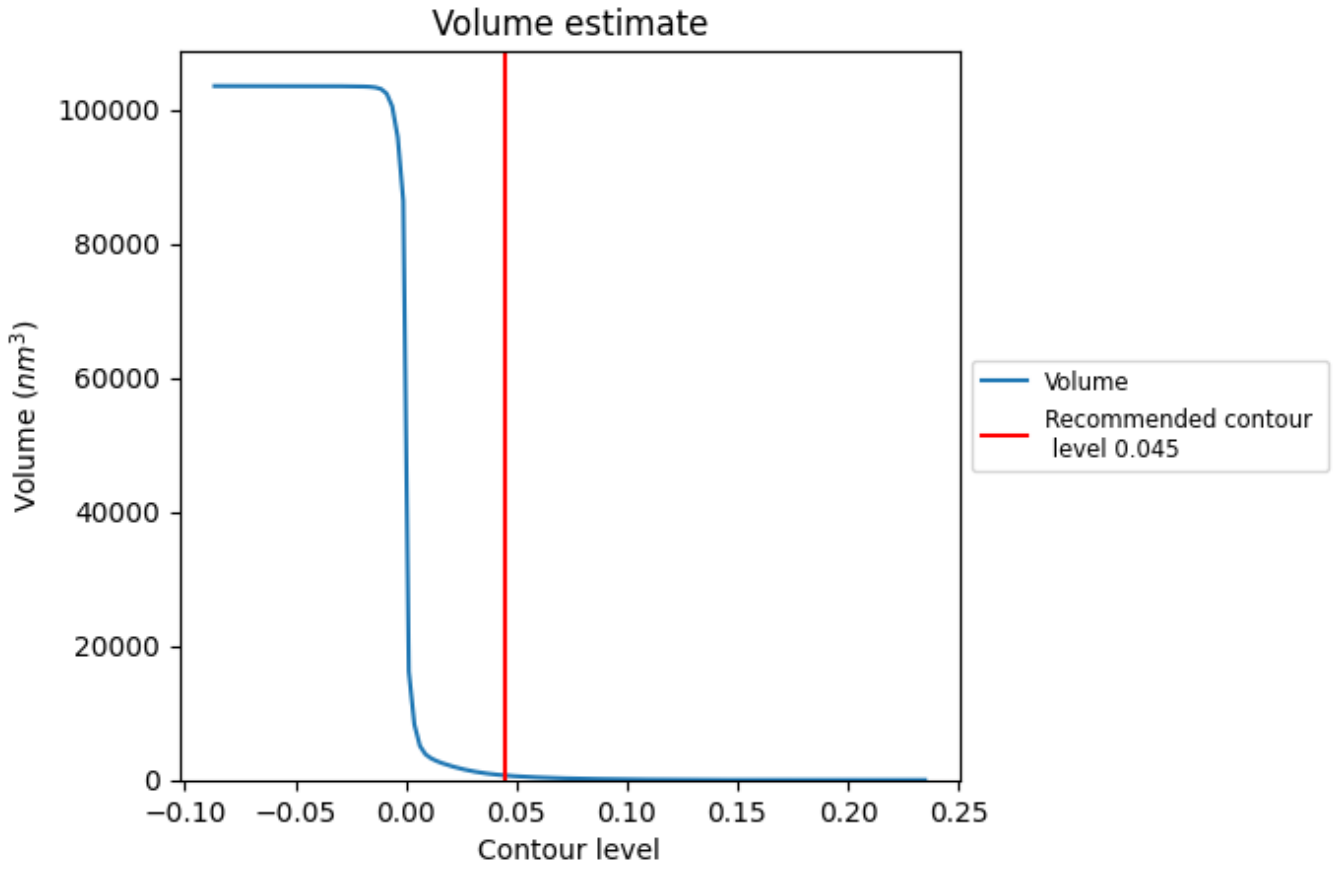
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

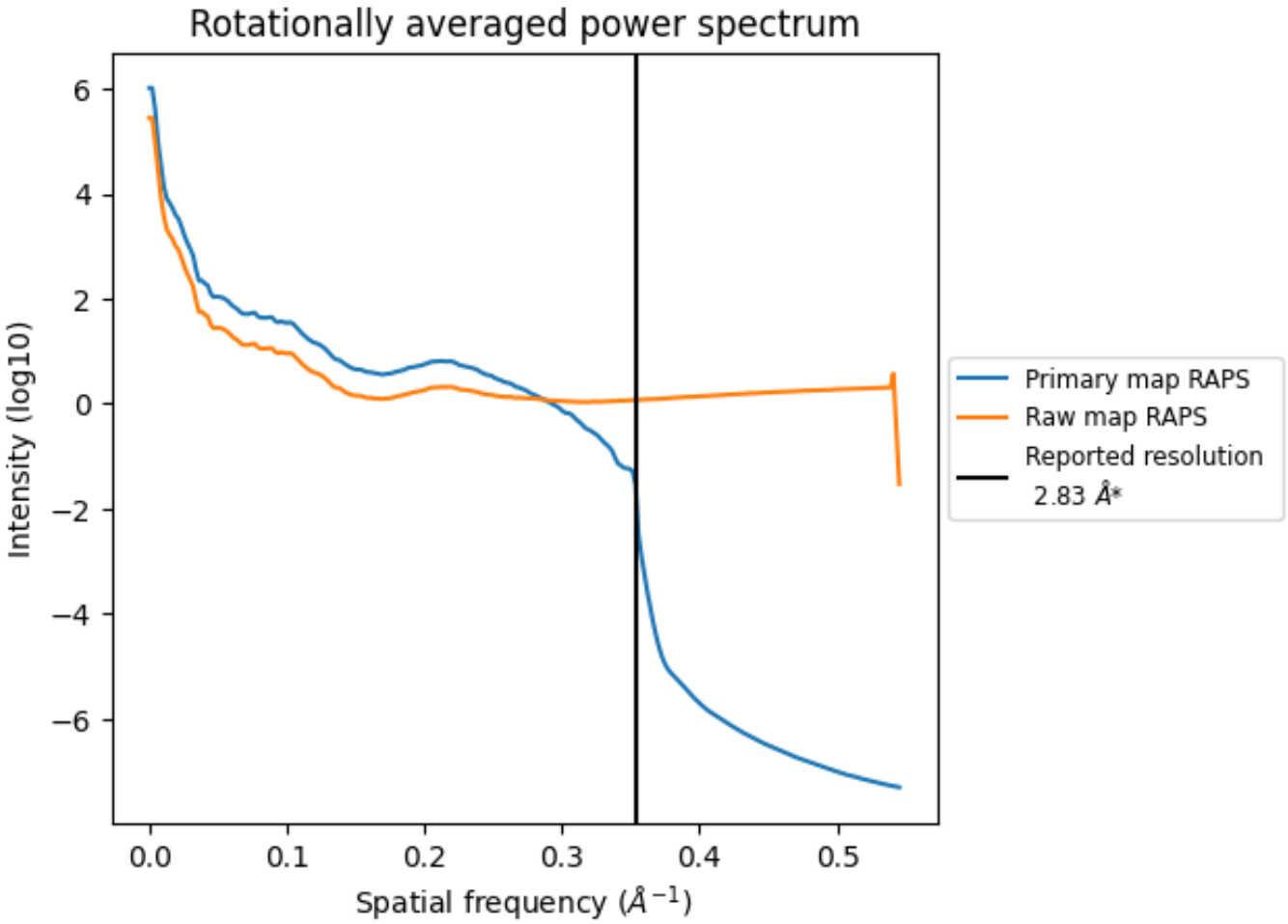
7.2 Volume estimate



The volume at the recommended contour level is 677 nm^3; this corresponds to an approximate mass of 611 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

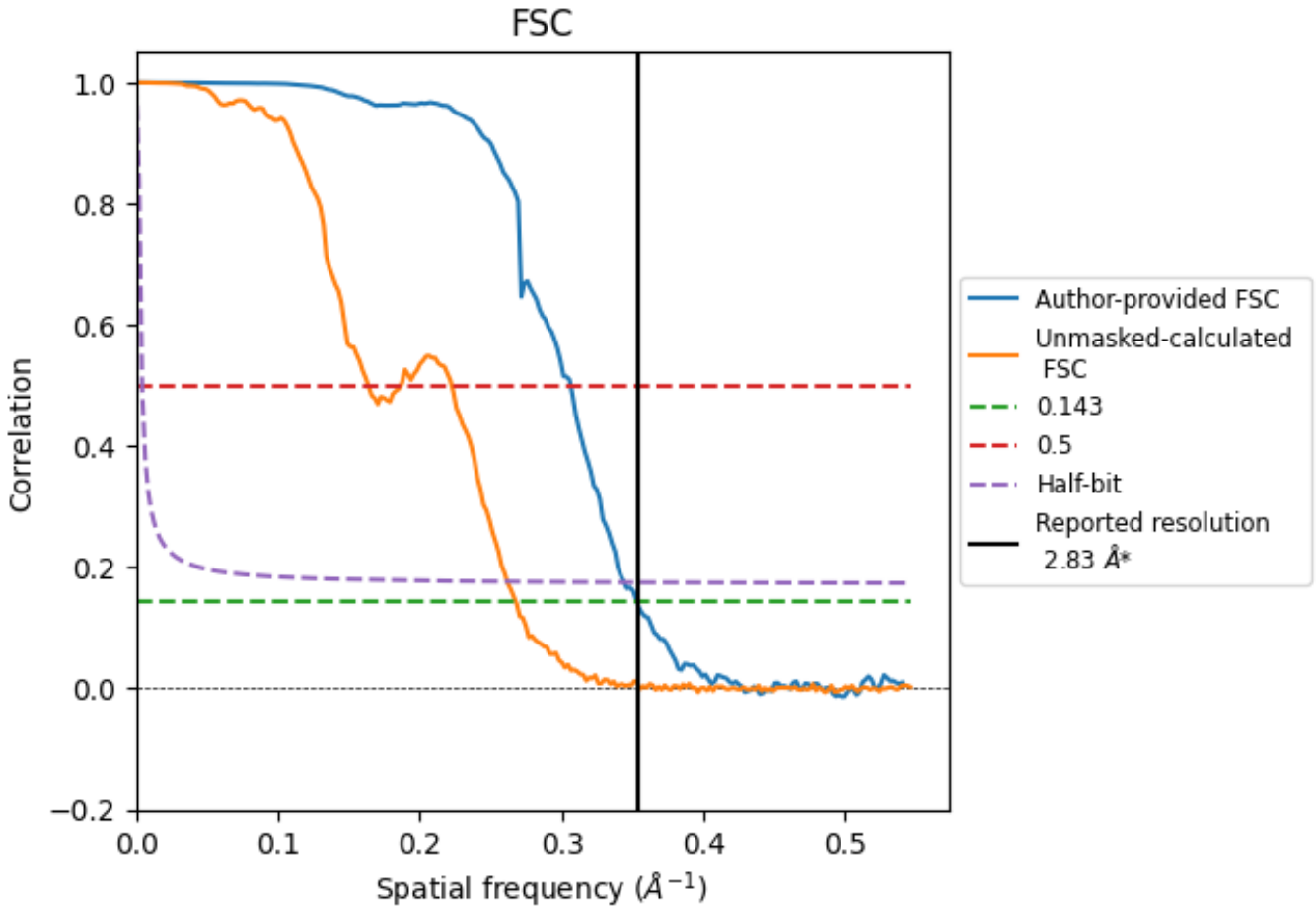


*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.353 Å^{-1}

8.2 Resolution estimates (i)

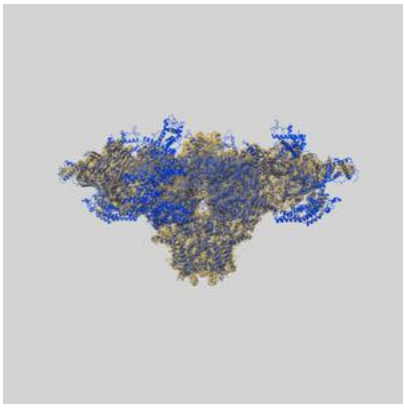
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.26	2.91
Unmasked-calculated*	3.74	6.11	3.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.83 by more than 10 %

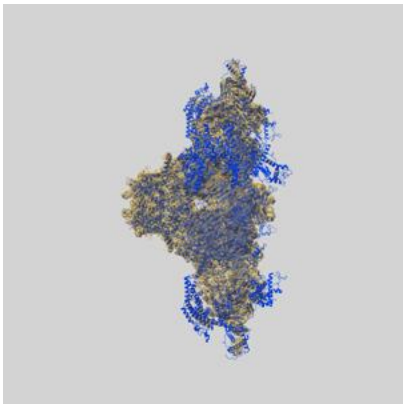
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80684 and PDB model 26IP. Per-residue inclusion information can be found in section 3 on page 12.

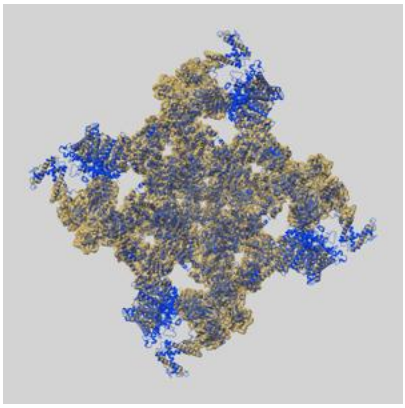
9.1 Map-model overlay



X



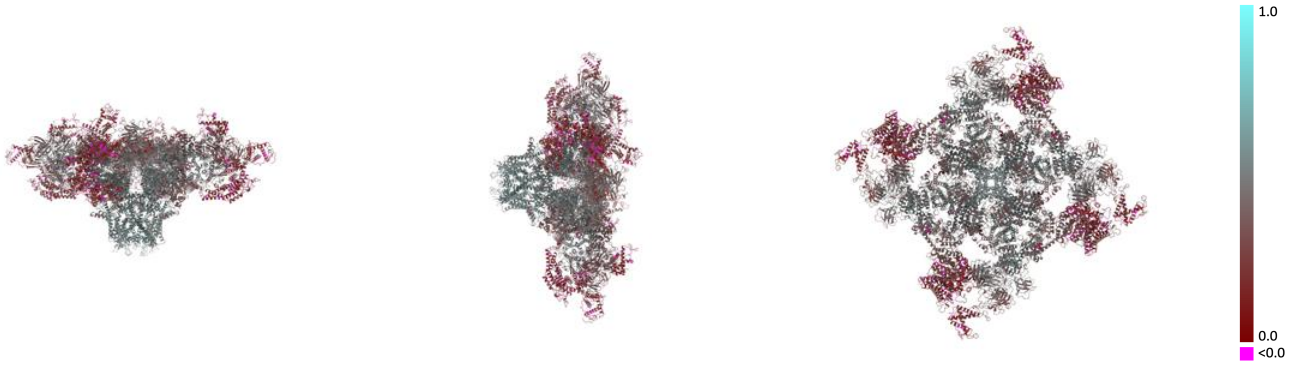
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

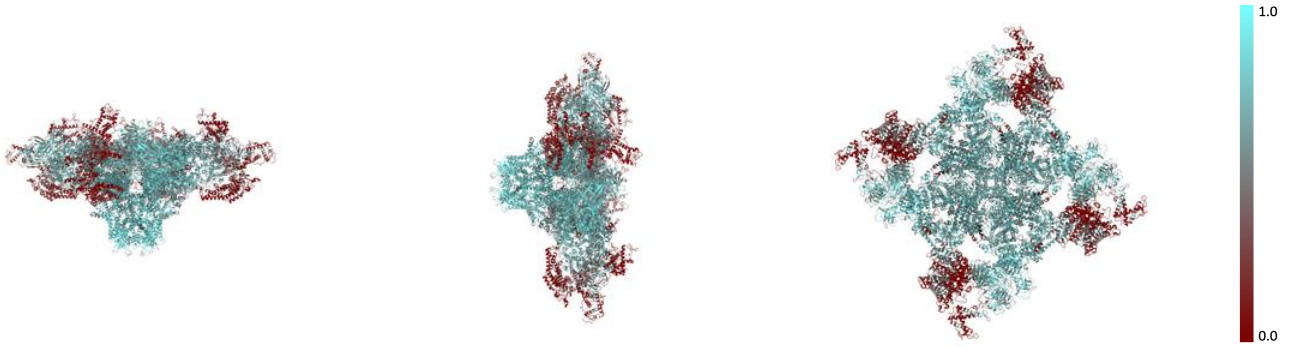
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

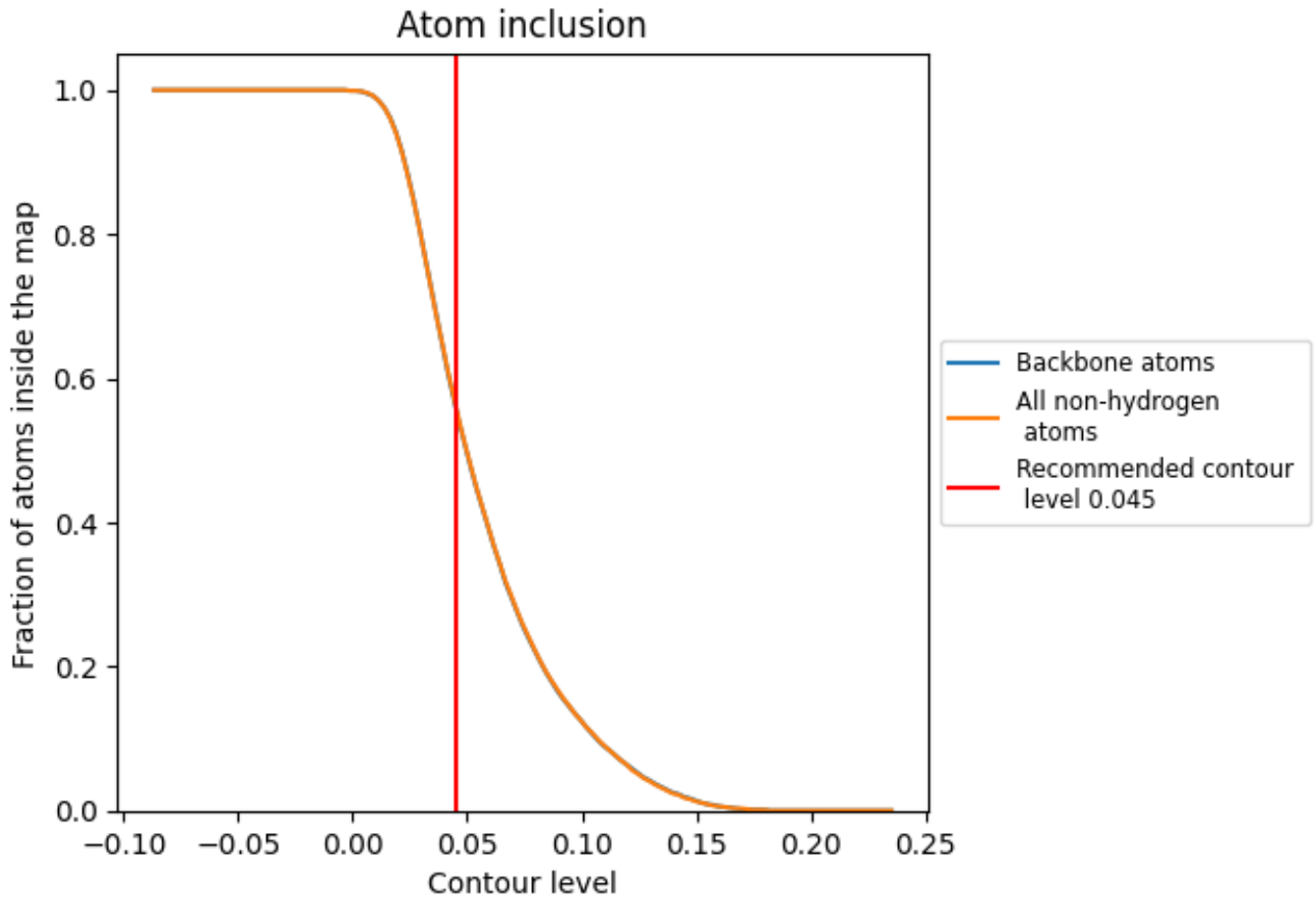
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5610	0.3740
A	0.5670	0.3730
B	0.5660	0.3730
C	0.5660	0.3730
D	0.5660	0.3730
G	0.7300	0.4320
H	0.7260	0.4310
I	0.7290	0.4340
J	0.7270	0.4340

